HYSPLIT Tutorial

Highlights 2020 Version 5.0.0

Introduction

- Everyone should have a video display to follow the on-line presentation ...
- and a computer to run simulations
- Primary focus will be on running examples through the GUI for novice users ...
- and a review of select scripted cases for more advanced users
- Many of the examples are designed to show the effect of various model settings
- In addition, several different real-world examples will be reviewed
- Start with single-particle trajectories and then expand to multi-particle dispersion

1.1 Windows PC HYSPLIT Install

- Install Tutorial
 - Copy or unzip file to c:\Tutorial, also contains meteorological data & examples
- Install HYSPLIT the first time on a clean PC
 - Install utilities (Tcl/Tk, Ghostscript, Ghostview, ImageMagick)
 - Download and run HYSPLIT_win64{R|U}_v5.0.0_rev????.exe
- Install on a PC with an older version already installed
 - Existing utility programs can be used with any version
 - Rename the old HYSPLIT directory (e.g. c:\hysplit_old)
 - Install new HYSPLIT
 - Renaming forces new code to reconfigure directories (default_exec)
- Hints
 - Create desktop shortcut to notepad
 - Show extensions for know file types

Utility Example: Installing ActiveState Tcl/Tk

- Go to: www.tcl.tk
- Get Tcl/Tk
- Binary Distributions
- ActiveTcl
- Create a free account to get ActiveTcl (must create a free account)
- Featured projects & languages
- ActiveTcl 8.6 Windows
- View all downloads
- Windows
- Download windows installer: Download.exe
- Downloads: ActiveTcl-8.6.9.8609.2-MSWin32-x64-5ccbd9ae8.exe
- Then, install, as instructed

1.2 Apple MAC OSX HYSPLIT Install

- Install Tutorial
 - Copy or unzip file to \${HOME}/Tutorial
- Install HYSPLIT the first time on a clean MAC
 - Install utilities (Tcl/Tk, ImageMagick)
 - Open the downloaded hysplit_v5.0.0.dmg
 - Run the Install_hysplit.app
 - This will copy the hysplit directory to your \$HOME directory (/Users/account/hysplit) and place the hysplit.app on your desktop
 - To allow apps downloaded from anywhere: sudo spctl --master-disable
 - You may need to customize default_exec:

#Xwindows_dir: /opt/X11/bin

#Image_Magick_pgm: /opt/local/bin/convert

- Install on a MAC with an older version already installed
 - Existing utility programs can be used with any version
 - Rename the old HYSPLIT directory (e.g. \${HOME}/hysplit_old)
 - Run the Install_hysplit.app

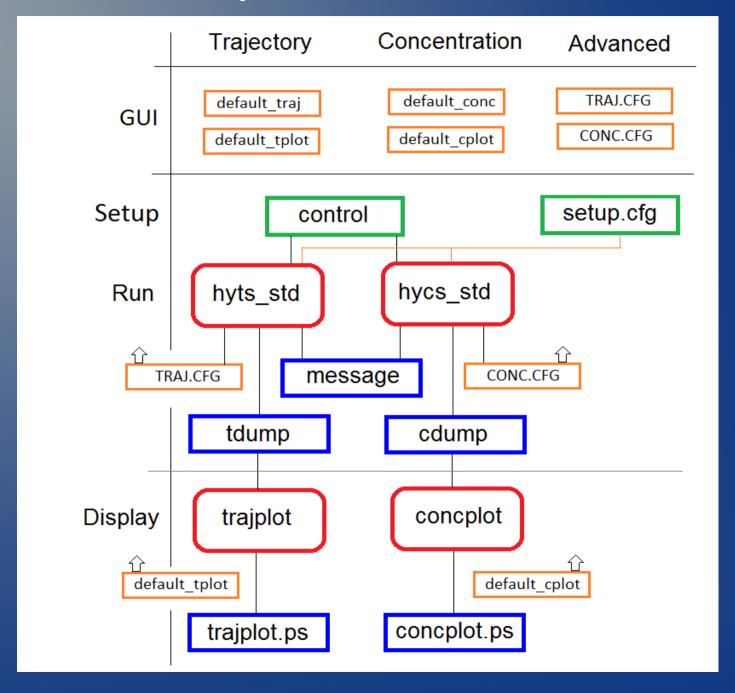
1.3 UNIX – LINUX HYSPLIT Install

- Install Tutorial
 - Copy or unzip file to \${HOME}/Tutorial
- Install HYSPLIT the first time on a clean computer
 - Install utilities (Tcl/Tk, Ghostscript, ImageMagick)
 - for commands: wish, gs, convert (check /usr/bin versus /usr/local/bin)
 - Install HYSPLIT from repository (follow emailed instructions)
 - https://svn.arl.noaa.gov:8443/svn/hysplit/tags/hysplit.vX.Y.Z
 - Edit Makefile.inc and follow compilation instructions
 - Create desktop icon: see /tutorial/bash/icon2desk.sh
- Install on a computer with an older version installed
 - Follow SVN update instructions (see script /hysplit/update.sh)

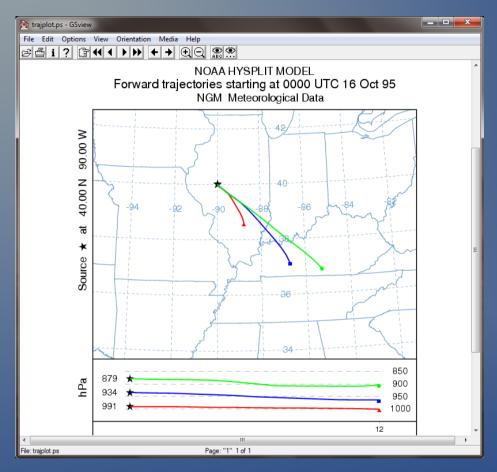
1.4 HYSPLIT Directories

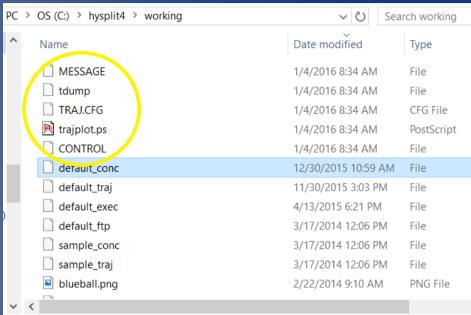
- data2arl: convert data to HYSPLIT format
 - Source code for MM5, WRFARW, ECMWF
- datem: data archive of tracer experiments and meteorology
 - Data for all CAPTEX releases plus many other experiments
 - https://www.arl.noaa.gov/research/dispersion/datem/
- exec: contains compiled executables
- document: detailed model description ARL-224.pdf
- graphics: map background files
- guicode: graphical user interface
- html: GUI context sensitive help files
- python: installation scripts for new display programs
- working: default location for model input and output
 - To launch HYSPLIT GUI from working: ..\guicode\hysplit.tcl

2.1 Graphical User Interface

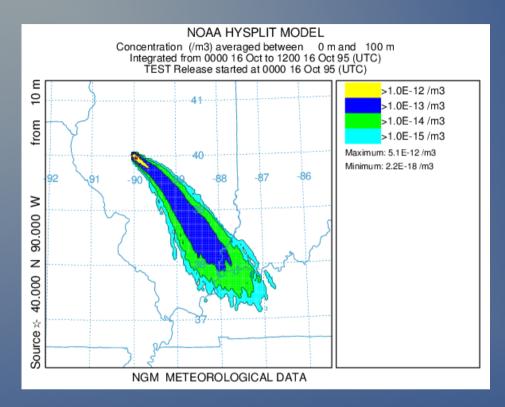


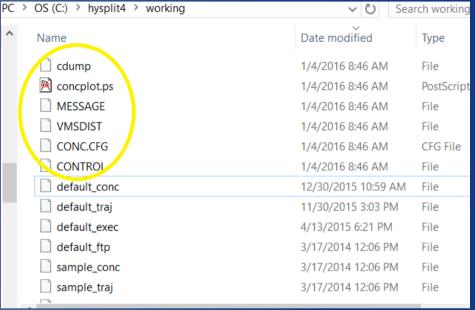
2.2 Test Trajectory Calculation



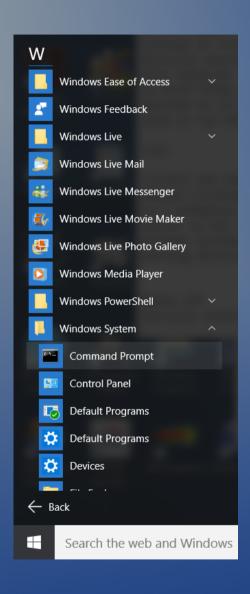


2.3 Test Air Concentration Calculation





2.4 Batch File Scripting

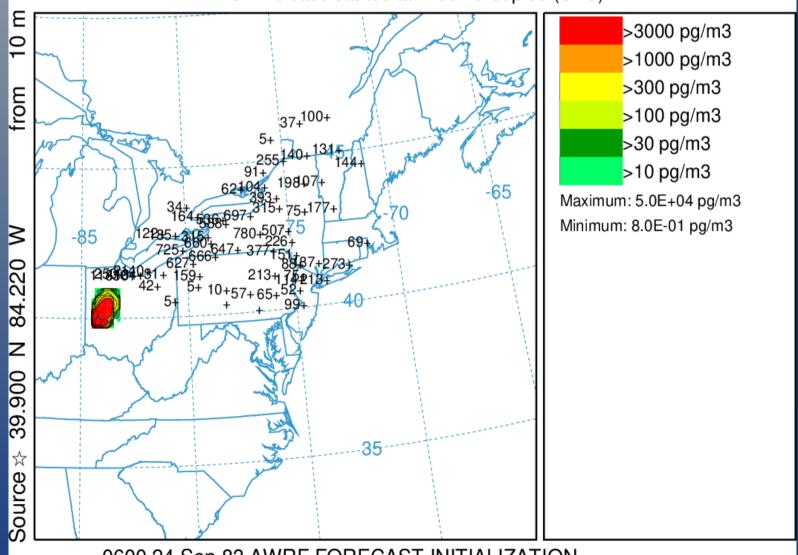


- Run for the first time
 - C:\Tutorial\batch\test_conc_bat
- Review results
 - cd \hysplit\working
 - dir
- Edit and rerun
 - notepad CONTROL
 - ..\exec\hycs_std
 - ..\exec\concplot –icdump
 - concplot.ps

2.5 Using CAPTEX Data

NOAA HYSPLIT MODEL

Concentration (pg/m3) averaged between 0 m and 100 m Integrated from 1800 25 Sep to 2100 25 Sep 83 (UTC) PMCH Release started at 1700 25 Sep 83 (UTC)

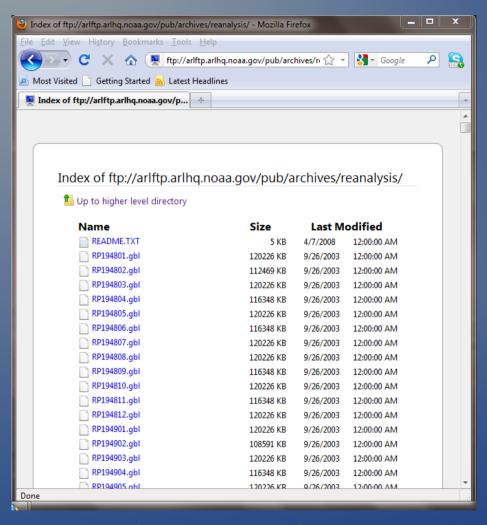


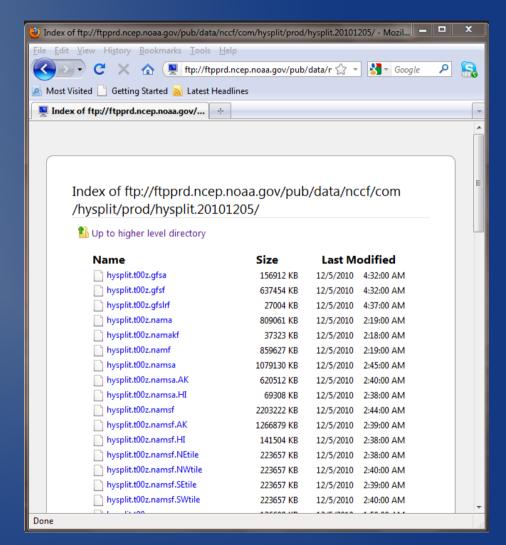
0600 24 Sep 83 AWRF FORECAST INITIALIZATION

3.1 HYSPLIT Meteorological Data

- A file contains data for one or more time periods
- Each time period consists of two types of fixed-length records (for direct access): header and data
 - The header record contains information about the grids and variables
 - The data records are one per variable and level
- Each data record contains
 - 50 bytes ASCII with time and level data
 - Followed by Number-X times Number-Y bytes of packed data
- Because of a mix of ASCII and binary data on each record never let the FTP client automatically decide on the mode
 - It should always be manually set to image or binary!
- Various HYSPLIT compatible data are provided for the tutorial
 - If accessed on-line, there are links to download the data files

3.2 FTP Meteorological Data or MAC=CMD+K





ARL for archives and forecasts

NCEP for forecasts

3.3 Convert Meteorological Data

- HYSPLIT requires meteorological data on an evenly spaced grid (latitude-longitude or conformal projection) at multiple heights and time periods over the duration of the simulation.
- The conversion process is complicated, it is best to use already formatted data if available!
- Conversion programs for multiple raw data formats are provided (in the data2arl directory):

NetCDF arw2arl, cdf2arl, mer2arl

■ GRIB-1 era52arl, grib2arl

GRIB2 api2arlMM5 mm5v3

- Although most data are well-documented (e.g. GRIB)
 - Variables and order within each file may vary
 - Temporal resolution and vertical coordinate system may differ
 - Perhaps even for the same model!
- Some customization may be required!

3.4 Meteorological Data Servers

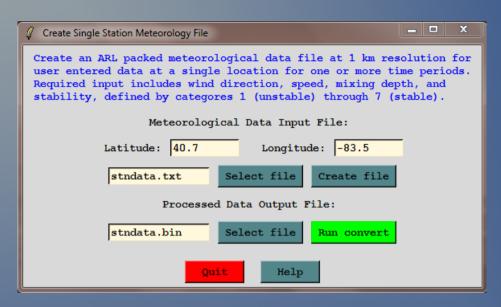
ARL <u>ftp://arlftp.arlhq.noaa.gov/pub/</u>

NCEP https://nomads.ncep.noaa.gov/pub/data/nccf/com/hysplit/prod/

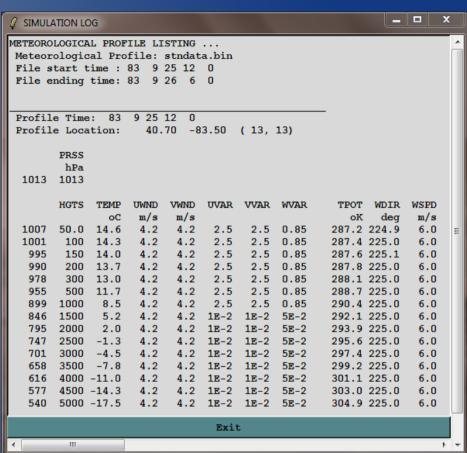
University of Alaska

Spain http://www.hyspli

3.5 User Entered Meteorological Data



- Program = STN2ARL
 - Same direction and speed for all levels and locations
 - Standard atmosphere temperature profile
 - Turbulence defined within mixed layer
- Program = SND2ARL
 - Define sounding at one location
 - Not available through the GUI



4.1 The Trajectory Calculation

83 09 25 17

39.90 -84.22 10.0

68

tdump

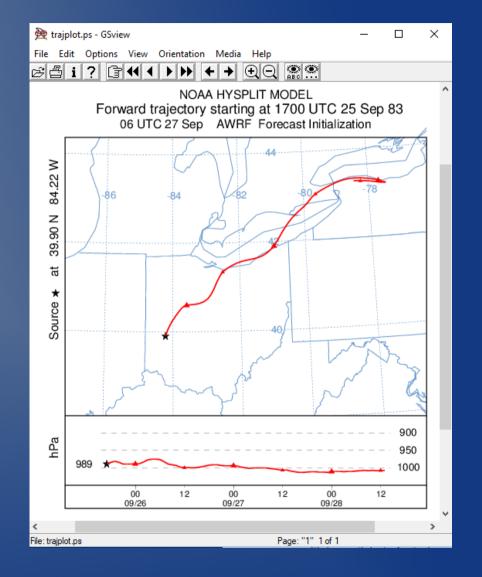
c:/Tutorial/captex/

captex2_wrf27uw.bin

start time
start location
run duration
output file
meteo directory*

meteo file

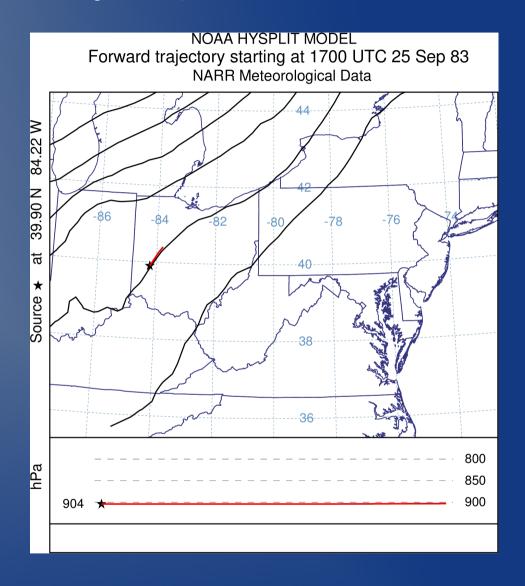
Example of how a single trajectory is insufficient to explain the large- scale tracer distribution seen in the earlier CAPTEX data animation.



^{*}Change default location

4.2 The Trajectory Equation

- $P'(t+\Delta t) = P(t) + V(P,t) \Delta t$
- $P(t+\Delta t) = P(t) + 0.5 [V(P,t) + V(P',t+\Delta t)] \Delta t$
- Δt (min) < 0.75 / Umax
- Horizontal in native input grid units
- Vertical coordinates transformed to
- $\sigma = (Ztop Zmsl) / (Ztop Zgl)$
- Ztop defaults to 25,000 m



4.3 Estimating Mixed Layer Depths

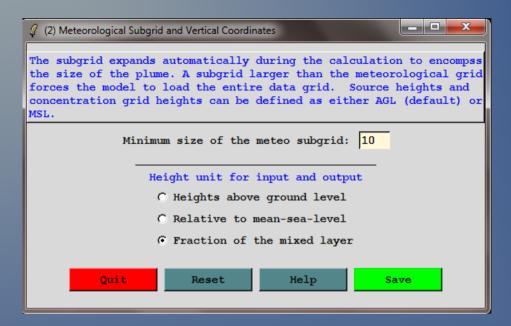
Review Problem #2 of Exercise #3

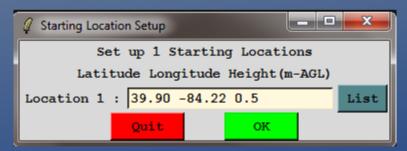
MSL	Pres	Temp	Dewp	Wdir	Wspd	Theta
m	hPa	K	K	deg	m/s	K
298	991	294.1	276.7	200	3.1	294.9
371	983	291.4	274.4			292.8
556				213	6.2	
864				223	5.7	
1172				229	5.7	
1419	868	282.6	269.8			294.3
1477				224	5.1	
1592	850	281.4	265.8			294.8
1739	835	281.9				296.8
1770				216	5.7	
2072	802	281.4		222	6.7	299.7
2361				230	7.7	
2622	750	277.7	268.7			301.5
2654	747	276.9	270.4	240	8.2	300.1

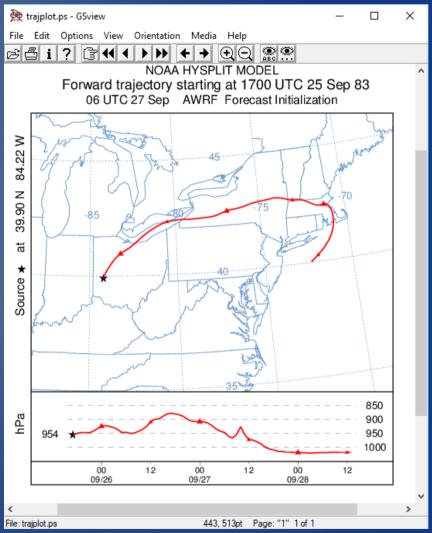
SIMU	LATION I	LOG											-		×	(
																٨
Profil	e Time	: 83	9 25	18 0				_								
Used N	earest	Grid	Point	(24,	24)	to Lat	: 3	9.90,	Lon:	-84.2	2					
	2D Fi	elds														
	SHGT	PRSS	TPP1	DIFR	PBLH		DSWF	SHTF	LHTF	T02M						
	m	hPa	mm		m	cm/s		W/m2		oC	m/s	m/				
988	320	988	0	0	1222	59.6	765	217	178	20.2	1.4	5.	0 203.	6 5.	. 2	
	3D Fi															
	PRES	TEMP	UWND	VWND	WWND	DIFW	SPHU q/kq	TKEN J/kg	DIFT			IR	w			
987	987	19.8	m/s 1.2	m/s 4.7	mb/h	-4E-6	g/kg 5.4		-1E-2		oK d .0 203	leg	4.8			
985	985	19.4	1.3		-2.0		5.4	1.2			.8 202		5.2			
983	983	19.1	1.3	5.1		-4E-6	5.4		1E-2		.7 202		5.3			
980	980	18.9	1.3	5.2		-1E-5	5.3		-4E-3		.7 202		5.4			
976	977	18.5	1.5		-1.9		5.3		-1E-2		.7 203		5.6			
971	972	18.0	1.5	5.4		4E-5	5.3		1E-2		.6 203		5.6			
966	967	17.7	1.5	5.5		-3E-5	5.3	1.4	1E-2	293	.6 204	.1	5.7			
961	963	17.3	1.6	5.6	-1.6	-4E-5	5.3	1.5	-2E-2	293	.7 204	.1	5.8			
954	956	16.7	1.7	5.6	-1.5	-1E-5	5.3	1.5	-1E-2	293	.6 204	.9	5.9			
944	948	15.9	1.8	5.7	-1.5	5E-5	5.3	1.6	1E-2	293	.5 205	.7	5.9			
934	939	15.1	1.8	5.8	-1.5	-1E-4	5.2	1.6	1E-2	293	.5 205	. 4	6.0			
924	930	14.3	1.9	5.8	-1.7	1E-4	5.2	1.6	1E-2		.5 206		6.1			
914	921	13.5	2.0	5.8	-2.1		5.2	1.6	1E-2		.5 207		6.2			
904	912	12.7	2.0	5.9		-2E-5	5.2	1.5			.6 207		6.3			
892	901	11.7	2.0	5.9		4E-6	5.1		-1E-2		.5 207		6.3			
877	887	10.4	2.1	5.9		-1E-4	5.1		-1E-2		.5 207		6.3			
862	874	9.2	2.2	6.0		2E-5	5.1		-4E-3		.4 208		6.4			
847 828	861 843	7.9	2.3 4.3	6.1 6.7	-5.3	-2E-5	5.1 3.3		1E-2 -2E-3		.4 208		6.5 8.0			
803	821	6.4	5.3	7.4		-1E-5	1.7	0	0		.7 224		9.2			
778	798	5.7	5.5			-1E-3	0.89	0	0		.5 223		9.6			
753	776	5.1	5.6		-5.8		1.0	0	0		.2 222		9.9			
726	752	4.1	6.2		-6.6		1.8	0	0		.8 226		10.1			
682	712	2.1	7.5		-6.4		2.7	ō	Ō		.4 237		9.9			
608	645	-2.0	10.4		-4.2		2.7	0	0		.3 248		12.0			
516	563	-8.4	10.2		-1.6	1E-4	2.5	0	0	312	.1 255	.8	11.1			
417	475	-16.4	9.6	0.14	-0.98	-1E-5	1.5	0	0	317	.8 277	.6	9.6			
306	375	-28.9	13.8	-5.3	-1.5	2E-5	0.59	0	0	323	.5 299	.5	14.8			
195	275	-45.6	30.2	-9.8	-0.51	-1E-5	0.14	0	0	329	.2 296	.5	31.8			
116	204	-58.5	34.8	-13.5	-0.16	-4E-6	3E-2	0	0	338	.1 299	.6	37.3			
							Exit									

PBLH = 1222 m + 320 m = 1542 m MSL Sounding PBL ~ 850 hPA, 1592 m, 295 K

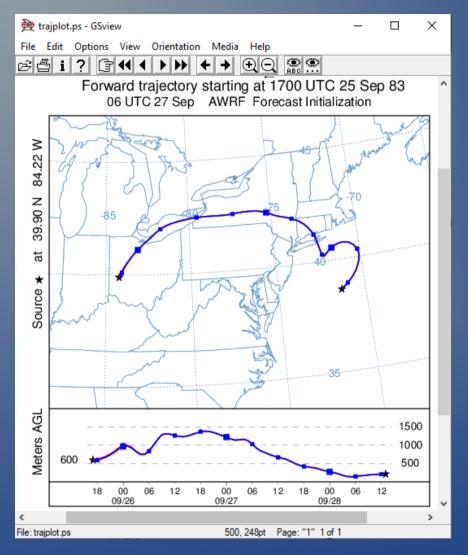
4.4 Mixed Layer Trajectories

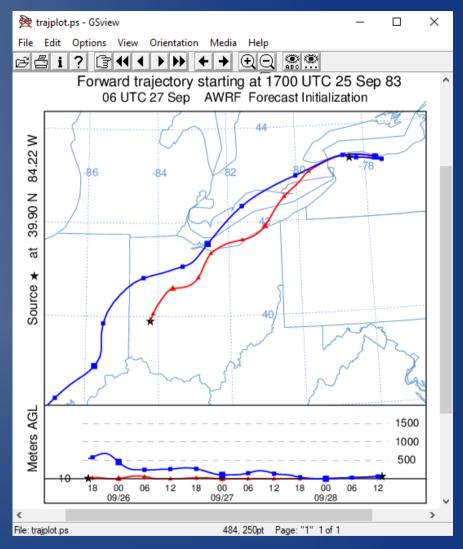




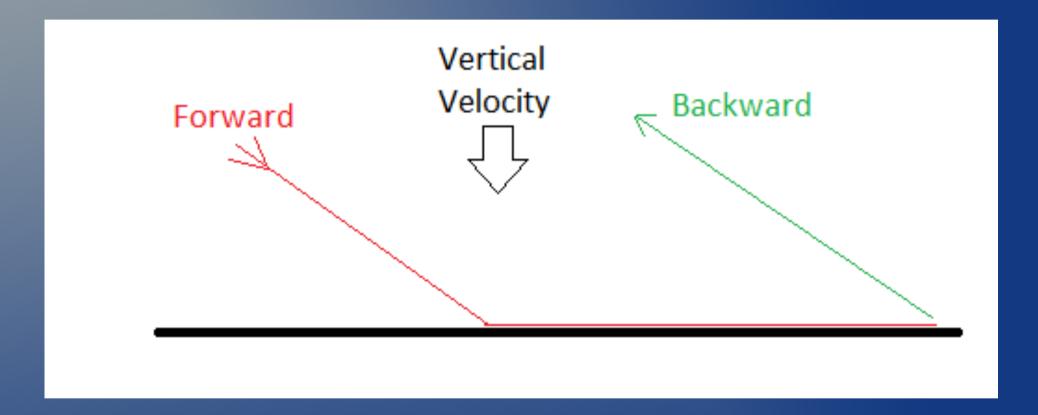


4.5 Computational Trajectory Error





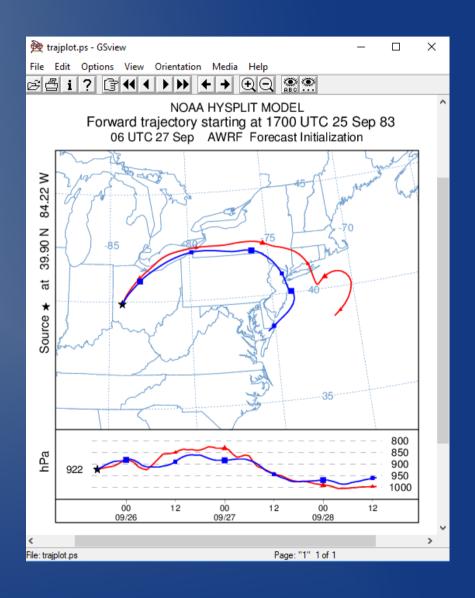
Computational Trajectory Error Terrain Effects



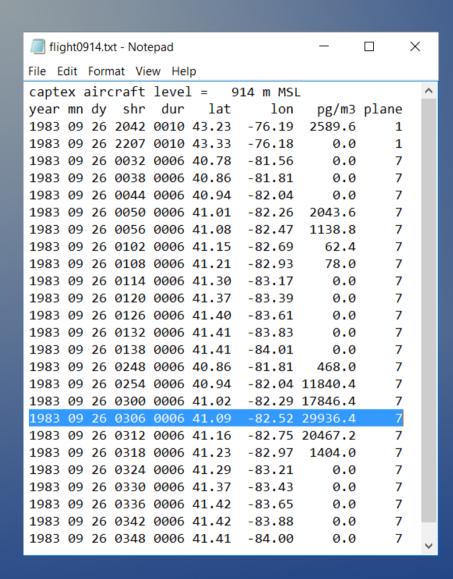
The backward trajectory at ground level does not know when the forward trajectory first intersected the ground due to downward motion.

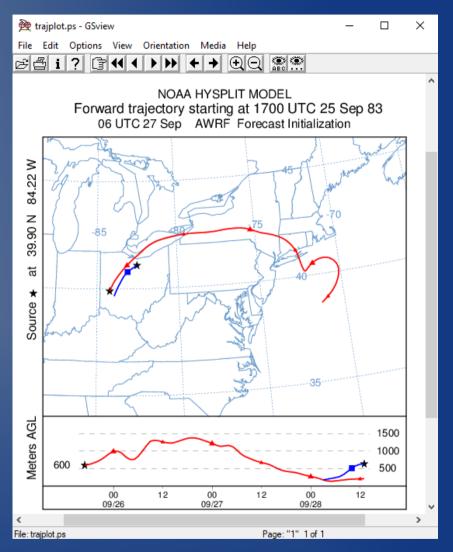
4.6 Meteorology Trajectory Error

- Trajectory = integration of position vector in velocity field
- Velocity field continuous in space and time
- Meteorological input data are discreet in space and time
- Discreet data are one of the primary sources of error!
- NARR and WRF shown in example



4.7 Absolute Trajectory Error

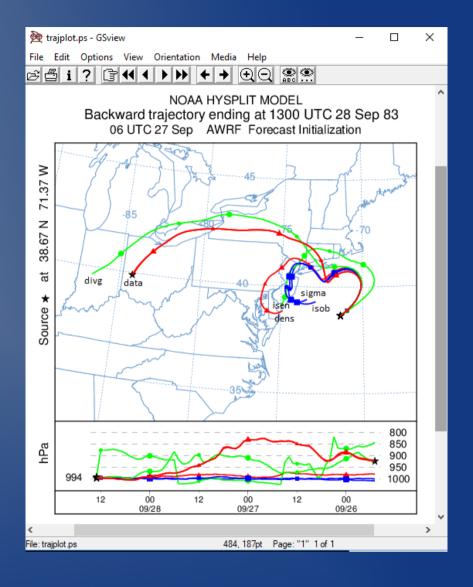




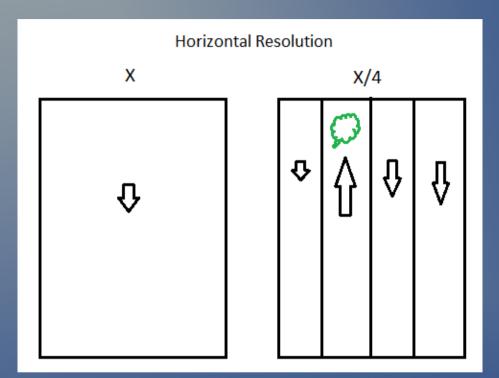
A backward trajectory from point of the maximum measured concentration should pass over the release location.

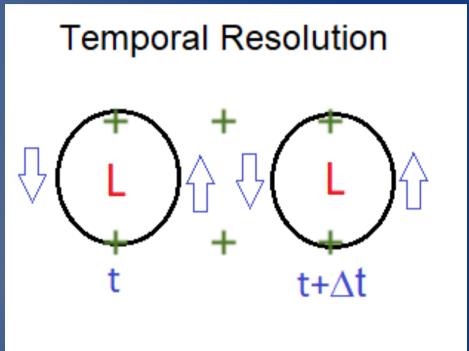
5.1 Trajectory Vertical Motion

- Wη = $(-\partial \eta/\partial t u \partial \eta/\partial x$ - $v \partial \eta/\partial y) / (\partial \eta/\partial z)$
- Options
 - Model data field (default)
 - Isobaric
 - Isentropic
 - Constant density
 - None (iso-sigma)
 - Divergence (default if data=none)
- W affected by ...
 - spatial resolution
 - temporal resolution (aliasing errors)



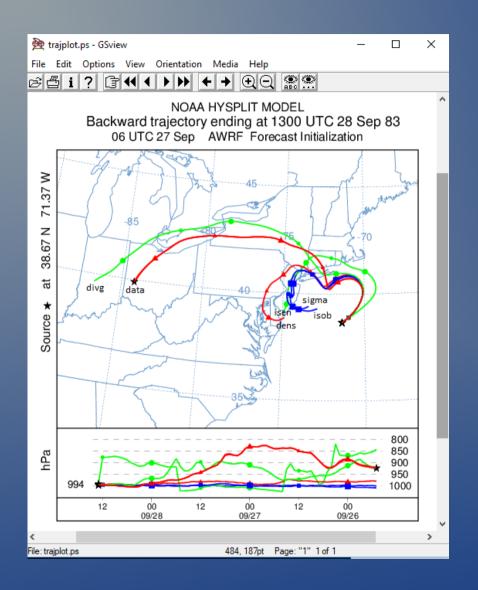
Spatial and Temporal Resolution

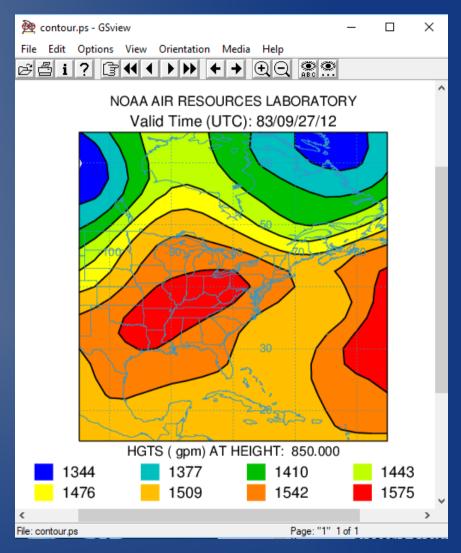




Large cell average velocity fields may not represent the true internal structure. For instance, clouds and rain may be a sub-grid scale feature. Too infrequent snapshots of the velocity field may not capture the finer time interval changes when intermediate values are interpolated between model output times.

5.2 Trajectory Flow Field

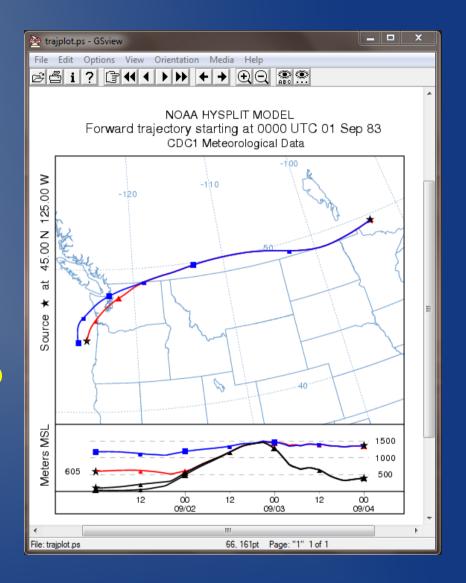




The flow field is not well defined at the backward starting location.

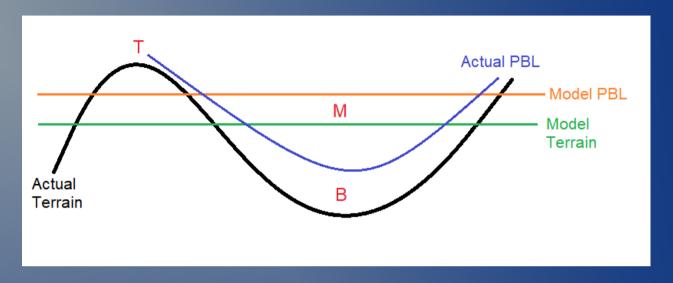
5.3 Trajectories and Terrain

- Trajectories that intersect the ground continue
- Trajectories that intersect the model top terminate
- The red forward trajectory rises with terrain
- The blue backward trajectory continues at the mountain top level
- Trajectories are fullyreversible except for those that intersect the ground



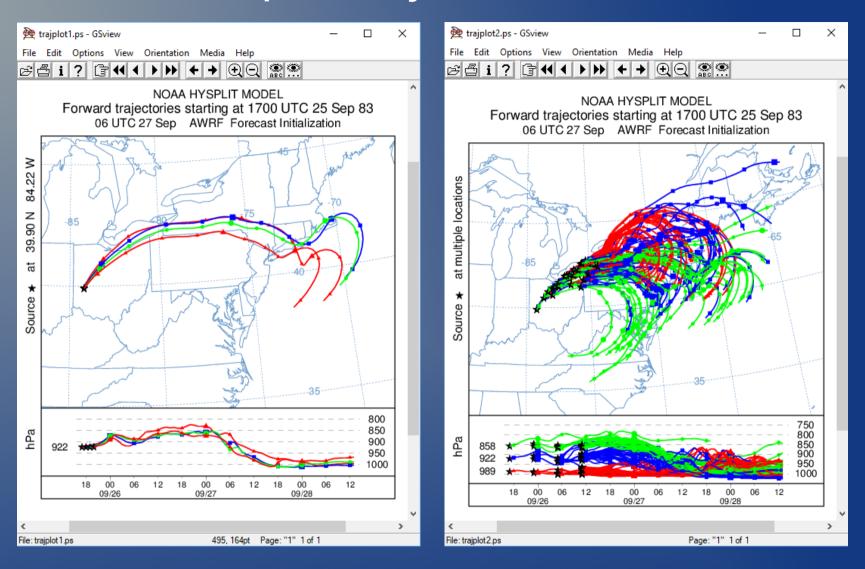
Trajectories and Terrain

Imperfect Options



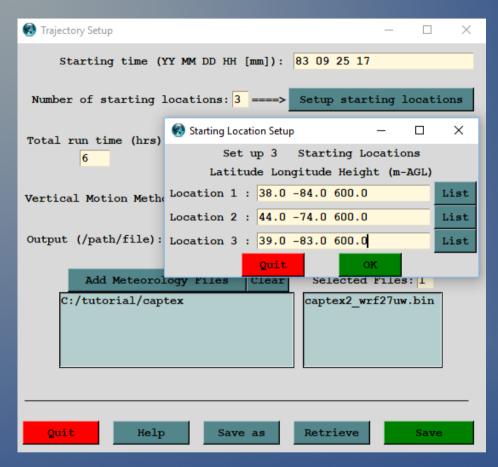
- Start trajectory at T from a height above model terrain corresponding to height of actual ground level above model terrain.
- Start trajectory at B from a height above the actual ground equal to a height above model terrain (M) so that it can be affected by PBL processes!

5.4 Multiple Trajectories in Time

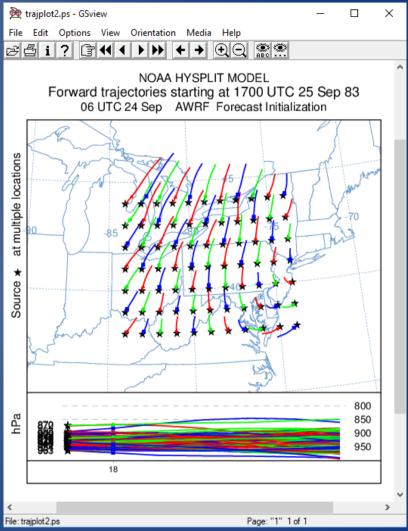


The surface tracer concentration distribution could be explained in large part by the changing wind directions with height and time within the mixed layer.

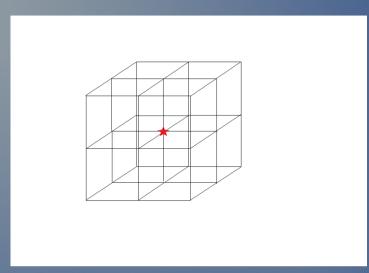
5.5 Multiple Trajectories in Space



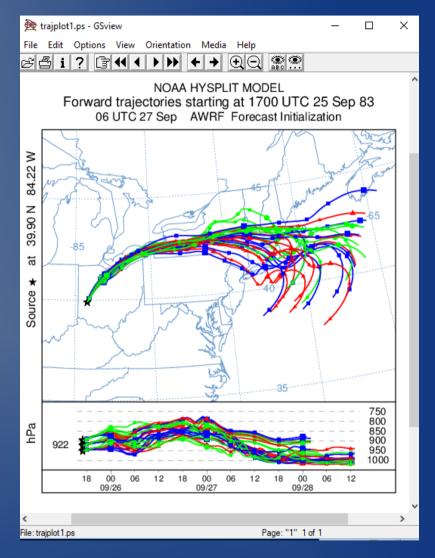
The trajectory matrix configuration shown in this section is a quick way to visualize the flow regime by creating many simultaneous trajectories.



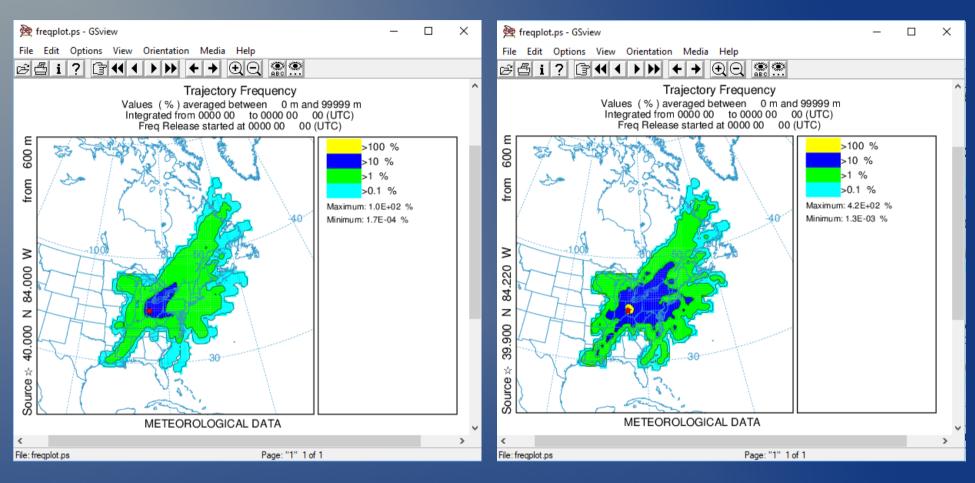
5.6 Meteorological Grid Ensemble



- Potential errors are large for a single trajectory due to errors representing a continuous field at discreet points (try the backward case)
- Use multiple trajectories in time or space to reduce uncertainty



6.1 Frequency Analysis



Only one count per trajectory

Fi,j = $100 \Sigma \text{ Ti,j} / \text{N}$

 Σ Ti,j ≤ 1.0

N = number of trajectories

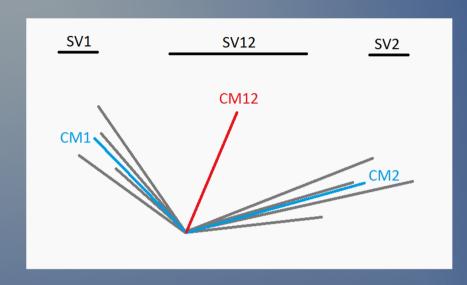
Count with Residence time

Fi,j = $100 \Sigma \text{ Ti,j} / \text{NP}$

 $\Sigma \text{ Ti, j} \leq P$

P = number of points per trajectory

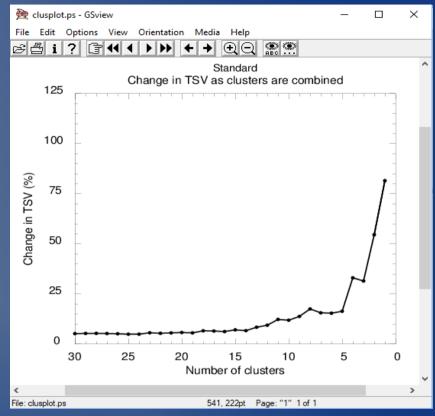
6.2 & 6.3 Cluster Analysis



Spatial Variance $SV_{i,i} = \Sigma_k (P_{i,k} - M_{i,k})^2$

Cluster Spatial Variance $CSV_i = \Sigma_i SV_{i,i}$

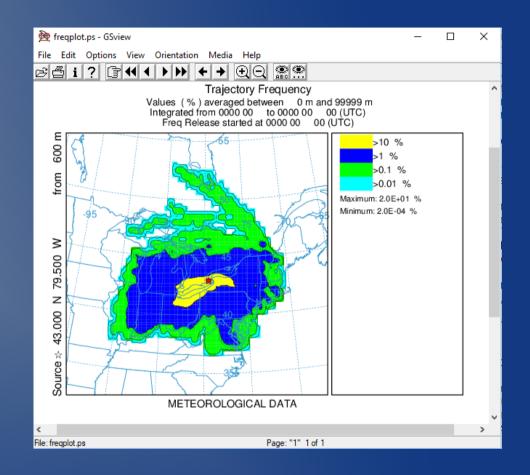
P = individual trajectory
M = cluster mean trajectory



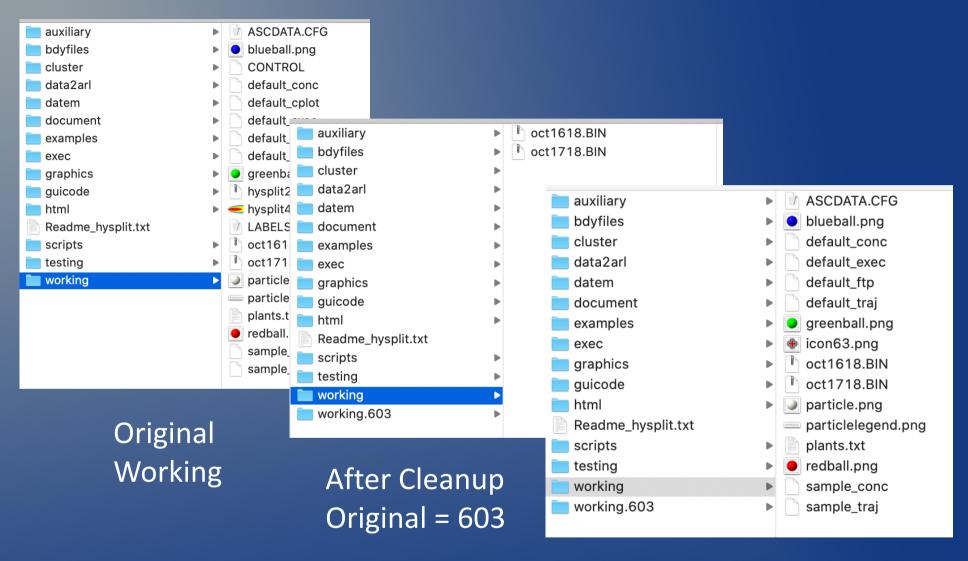
Total Spatial Variance $TSV = \Sigma_i CSV_{j,k}$

6.4 Source Geolocation

- Run backward trajectories from various locations corresponding with high measured values
- By superimposing these trajectories it may be possible to determine the source location
- For a more accurate geo-location, it is necessary to sample a variety of different flow orientations

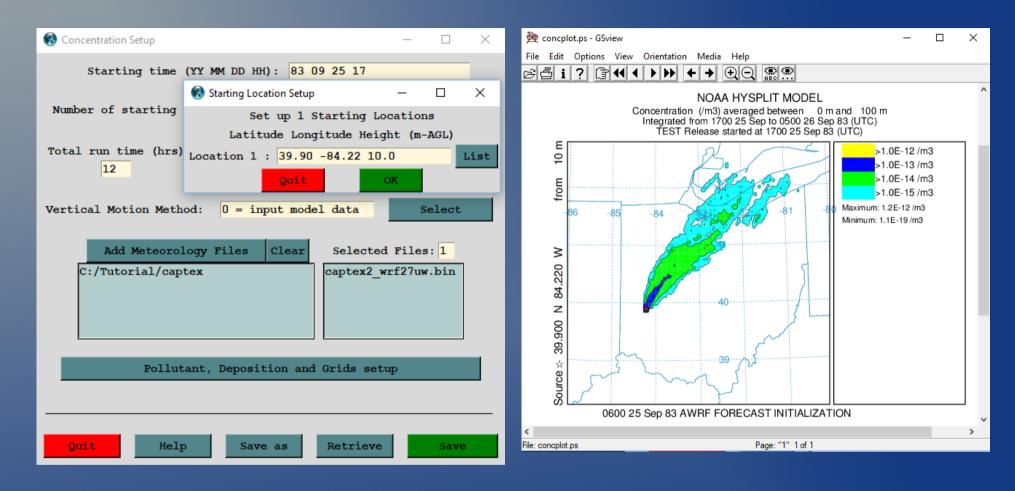


6.6 Working Directory Cleanup



After HYSPLIT GUI restart Replace default_exec?

7.1 Reconfiguring the Test Case



If one particle (mass = 1/2500) were contained in a grid cell of volume 5x5x1 km (2.5E+10 m³), then the air concentration would be about 1E-14 units m⁻³, a number comparable to the lower end of the range shown in the calculations

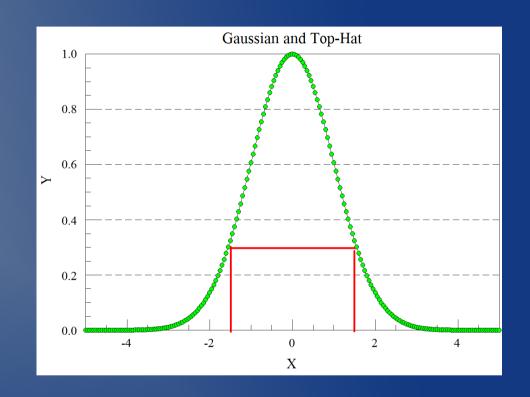
7.2 Air Concentration Equations

- Define Turbulence
 - U(t) = U'(t) + Ubar
 - U'(t) = U(t) Ubar
 - $\sigma_{II} = (1/n \Sigma U'(t)^2)^{0.5}$
- Turbulent displacement added to mean trajectory
 - $P(t+\Delta t)_{final} = P(t+\Delta t)_{mean} + U'(t+\Delta t) \Delta t$
- Turbulent velocity depends upon previous value
 - $U'(t+\Delta t) = R(\Delta t) U'(t) + U'' (1-R(\Delta t)^2)^{0.5}$
 - $R(\Delta t) = \exp(-\Delta t / TL)$
- Computer generated Gaussian random number: λ
 - U" = σ_{..} λ
- Turbulence statistic (assume $\sigma_{ij} = \sigma_{v}$)
 - From observations: $\tan \sigma_{\theta} = \sigma_{v} / u$
 - From model derived stability (Equations Section 9.3)

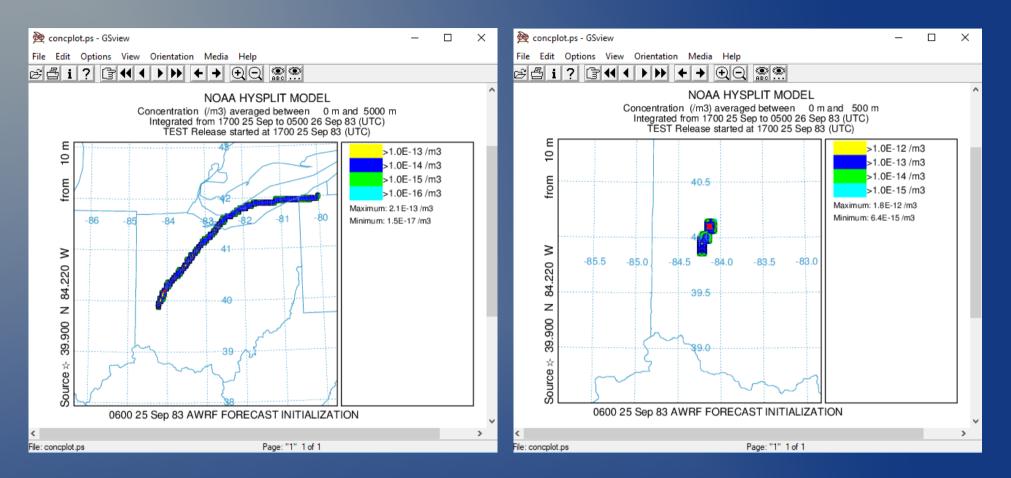
Air Concentration Equations

(sum particle trajectories to a grid)

- 3D Particle Model
 - $\Delta c = m (\Delta x \Delta y \Delta z)^{-1}$
- Puff particle distribution
 - $d\sigma_h/dt = \sigma_u$
- Top-Hat Puff ($r = 1.5 \sigma$)
 - $\Delta c = m (\pi r^2 \Delta z)^{-1}$
- Gaussian Puff (3 σ)
 - $\Delta c = m (2 \pi \sigma_h^2 \Delta z)^{-1} \exp(-0.5 x^2/\sigma_h^2)$



7.3 & 7.4 Single Particle Trajectory

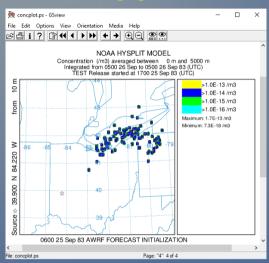


0 – 5000 m layer

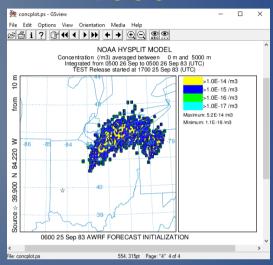
0 – 500 m layer

7.5 Releasing Multiple Particles

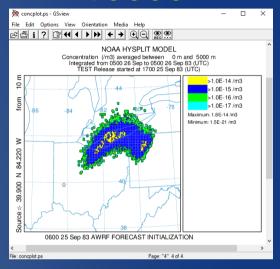
100



1000

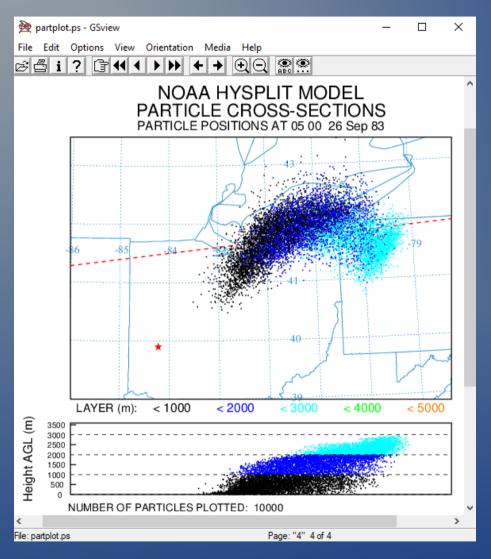


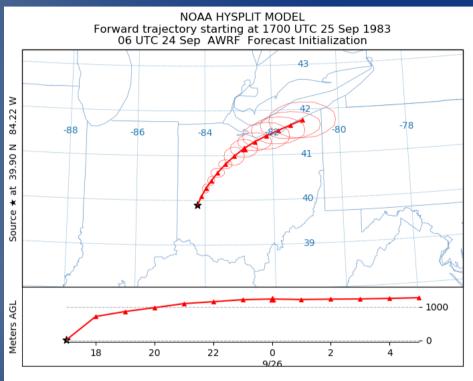
10000



- Simulations with various particle number release rates show that more particles are required for more realistic and detailed simulations (finer resolution grids)
- Realism comes with the cost of increased computational time
- This may become especially significant for continuous releases

7.6 Display Particle Positions

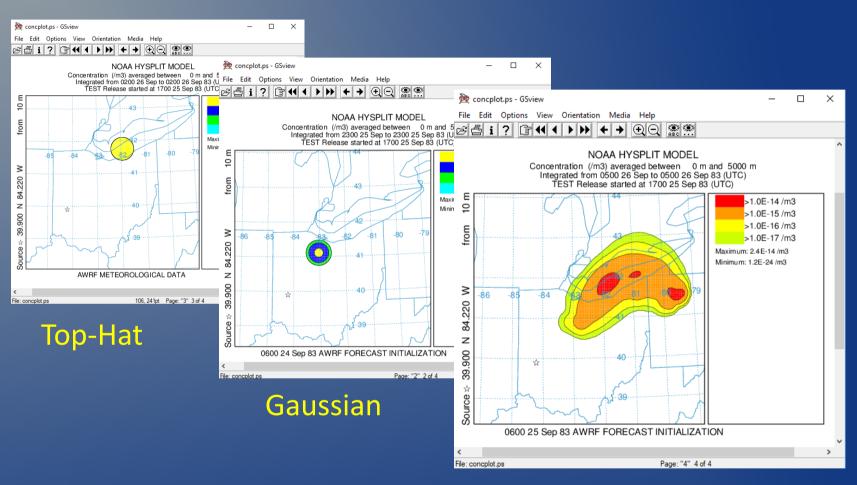




The center-of-mass trajectory requires the installation of Python

7.7 Particle Distributions using Puffs

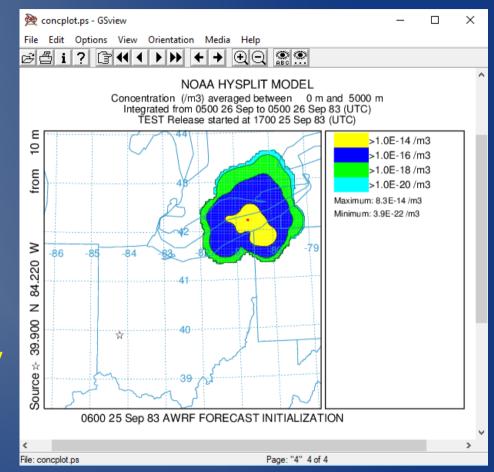
Modeling the distribution requires fewer computational particles



100 Gaussian

7.8 Downwind Puff Splitting

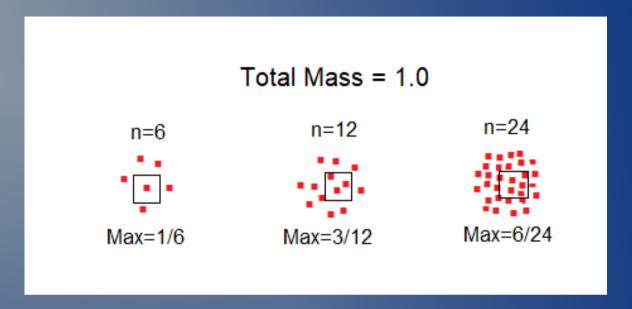
- Improves the representativeness of modelled flow over a single puff
- Results in an ever-increasing number of puffs
- When NPUFF>0.5*MAXPAR, puff splitting is turned off
- When NPUFF>MAXPAR, emissions (emit new puffs) are turned off
- If this occurs, air concentrations may be under-predicted
- Address by increasing the value of MAXPAR



Particles versus Puffs

- 3D particles provide better representation of a complex atmosphere
- The relation between particle number and grid size must be considered
- For puffs, splitting may become an issue
- If puff number exceeds maximum, emissions are shutdown
- The HYSPLIT default is the 3D particle mode
- Requires user to define the particle number requirements rather than relying upon puff-splitting to smooth the distribution

Exercise #7



- A finer concentration grid requires more particles ...
- Or fewer particles could utilize a coarser grid
- Particle number versus grid size sensitivity can be evaluated using the maximum concentration
- Minimum concentrations are also affected because the lower limit is the mass of one particle divided by the grid cell size
- This may be important if detection thresholds are a consideration in the model results

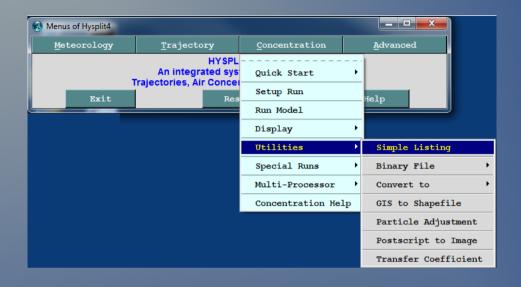
8.1 Configure for CAPTEX Release #2

- Total mass / number of particles released = mass per particle
- Particle mass contributing to a grid cell is summed over the "sampling" period
- A particle is a computational particle, it may represent a gas or particle
- One computational particle represents many billions of pollutant molecules (Avogadro's # 6x10²³)
- Mass of input units = output units: g/h → g/m³
- Units only matter when doing mass conversions

8.2 Air Concentration Display Options

- Air concentration
 - concplot map optimization and interpolation
- Particle position display
 - parxplot cross-sections
 - parhplot horizontal plane projection
 - parvplot vertical meridional and longitudinal
- Time-of-arrival
 - isochron arrival times at grid cell locations
- Grid point values
 - gridplot values at grid points (no interpolation)
- Polar-coordinate grid
 - poleplot requires special radius and distance grid

8.3 Air Concentration Utilities





- conread
 - Simple listing of concentration file contents

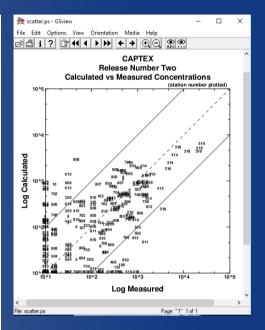
- con2asc
 - Import output to GIS
- con2stn
 - Time series at location
 - Input file of locations
 - Enter single point (X11?)
- timeplot
 - Used to display con2stn

8.4 Air Concentration Statistics

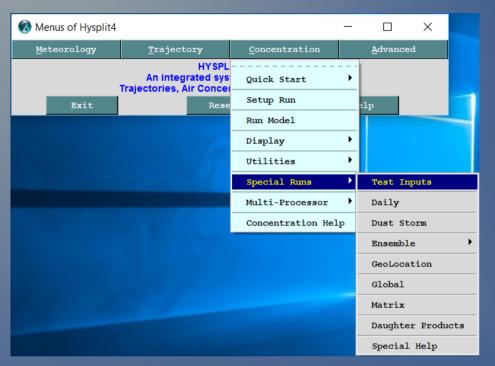
https://www.arl.noaa.gov/research/dispersion/datem/

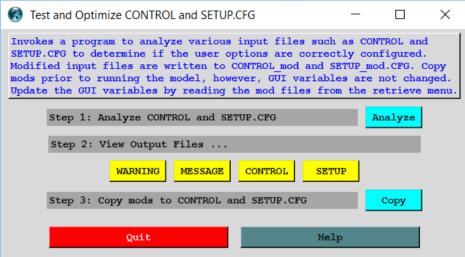
```
aptex2 meas.txt - Notepad
File Edit Format View Help
CAPTEX Release Number Two
year mn dy shr dur lat
                                    pmch stn
1983 09 26 0000 0300 40.38 -80.63
                                     .0 306
1983 09 26 0000 0300 40.77 -80.75
1983 09 26 0000 0300 40.92 -81.43
                                      .0 310
1983 09 26 0000 0300 41.30 -81.15
                                     .0 312
1983 09 26 0000 0300 41 42 -81 87
                                      0 314
1983 09 26 0000 0300 41.30 -82.22
                                   686.4 316
1983 09 26 0000 0300 41.27 -82.62 3556.8 318
1983 09 26 0000 0300 41.33 -83.12
                                   31.2 320
                                     .0 502
1983 09 26 0000 0600 40.20 -78.25
1983 09 26 0300 0300 40.38 -80.63
                                     .0 306
1983 09 26 0300 0300 40 77 -80 75
                                     0 308
1983 09 26 0300 0300 40.92 -81.43
                                   93.6 310
1983 09 26 0300 0300 41.30 -81.15
                                      .0 312
1983 09 26 0300 0300 41.42 -81.87 1357.2 314
1983 09 26 0300 0300 41.30 -82.22 4570.8 316
1983 09 26 0300 0300 41.27 -82.62 21028.8 318
1983 09 26 0300 0300 41.33 -83.12
                                   31.2 320
1983 09 26 0300 0600 40.00 -79.08
1983 09 27 0900 0600 40.37 -75.93
1983 09 27 0900 0600 40.78 -74.67
                                   312 0 703
1983 09 27 0900 0600 41.02 -75.90
                                   343.2 704
1983 09 27 0900 0600 41.83 -75.87 1497.6 706
1983 09 27 0900 0600 42 45 -76 45
                                  717 6 708
                                     .0 752
1983 09 27 0900 0600 43.98 -77.22
1983 09 27 0900 0600 44.28 -77.78
1983 09 27 0900 0600 39.93 -74.70
                                    62.4 802
1983 09 27 0900 0600 40.45 -74.80
                                   62.4 803
1983 09 27 0900 0600 40 90 -74 60
                                  234.0 804
1983 09 27 0900 0600 41.30 -74.67
                                  312 0 805
1983 09 27 0900 0600 41.63 -74.80
                                   483.6 806
1983 09 27 0900 0600 42.08 -74.97
                                   608.4 807
1983 09 27 0900 0600 42.47 -75.07 1123.2 808
                                  655.2 810
1983 09 27 0900 0600 43.23 -75.40
1983 09 27 0900 0600 43 58 -75 52
                                  109 2 811
1983 09 27 0900 0600 44 48 -76 03
                                     .0 852
1983 09 27 0900 0600 40.67 -73.52
                                   296.4 902
1983 09 27 0900 0600 41.27 -73.80 280.8 904
```

```
C:\Workshop results file: statA wrf27uw.txt
Model variation:
                 Tracer number: 0 Station select: All
      395 Unaveraged data points for processing
     0.00 Percentile input for zero measured
     0.00 Zero measured concentration value
     0.83 Correlation coefficient (P=99%)
    0.33 Regression Slope
    29.69 T-value (|Slope|/Standard Error)
   458.96 Average measured concentration
   296,80 Average calculated concentration
     0.65 Ratio of calculated/measured
    16.84 Normalized mean square error
  1514.64 Root mean square error
      395 Number of pairs analyzed
  -162.15 Average bias [(C-M)/N]
  -357.89 Lo 99 % confidence interval
    33.59 Hi 99 % confidence interval
    -0.43 Fractional bias [2B/(C+M)]
    16.37 False Alarm Rate [fa/(fa+hit)]
    71.86 Probability of Detection [hit/(hit+miss)]
    63.00 Threat Score [hit/(fa+hit+miss)]
    63.00 Fig of merit in space (%)
   -26.46 Factor exceeding [N(C>M)/N-0.51
    12.66 Percent C/M + 2
    28.86 Percent C/M ± 5
    31.65 Percent C/M ±10
    36.20 Percent M>0 and C>0
    14.18 Percent M>0 and C=0
    49.62 Percent M=0 and C>0
  1450.80 Measured 95-th percentile
   733.20 Measured
                   90-th percentile
   218.40 Measured 75-th percentile
   15.60 Measured 50-th percentile
  1543.53 Calculated 95-th percentile
   763.86 Calculated 90-th percentile
   188.76 Calculated 75-th percentile
     0.00 Calculated 50-th percentile
     9.00 Kolmogorov-Smirnov Parameter
```



8.5 Test and Optimize Input Files

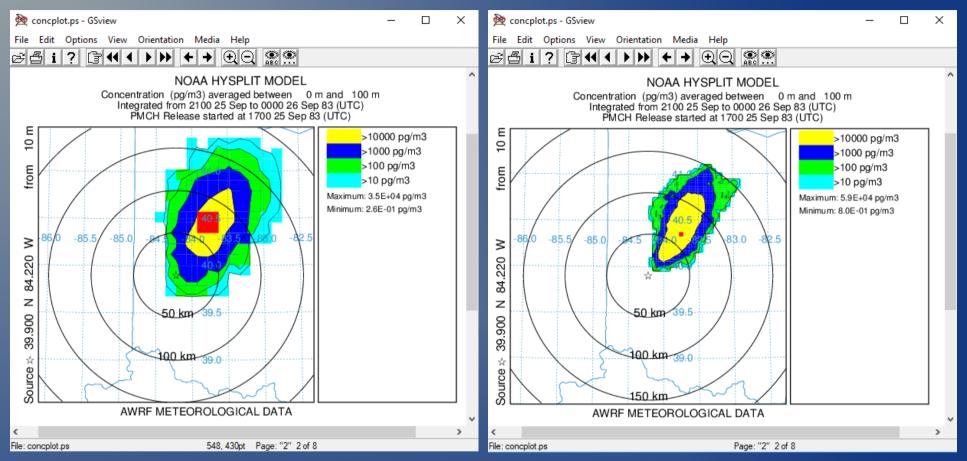




- Runs HYSPTEST, which is a simplified version of HYSPLIT
- Reads various input files and determines if user options are correct
- The program releases, transports, and disperses particles in the same manner as a regular simulation, except only one particle is processed
- If needed, modifications to CONTROL and SETUP.CFG are suggested

8.6 Simultaneous Multiple Grids

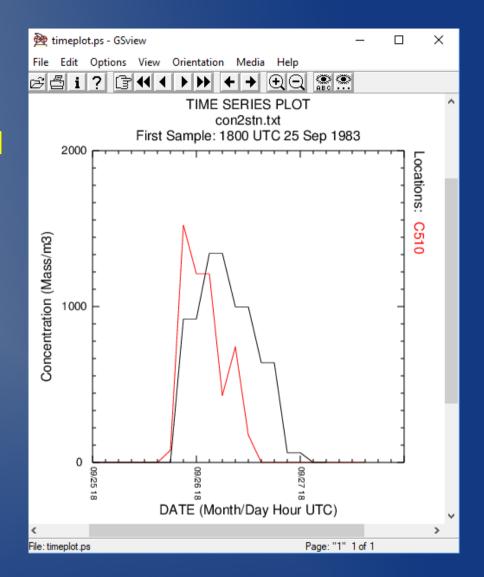
0.25 deg 0.05 deg



- For multiple meteorology grids, computations use only one grid per time step
- For multiple concentration grids, particles contribute mass to all grids
- Finer grids need more particles; shorter run duration requires fewer particles

Exercise #8

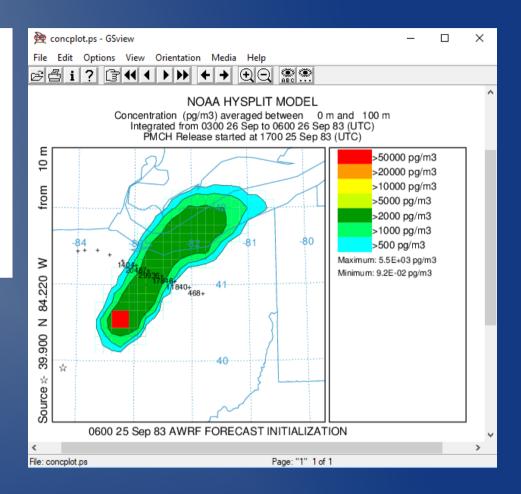
- Requires too much time to do both examples
- Show results from problem #1
 - Finer concentration grid does not mean better results
- Run problem #2, if sufficient time is available to complete
 - Finer meteorology grid does improve simulation!
 - Preconfigured script available



9.1 Case Study Base Configuration

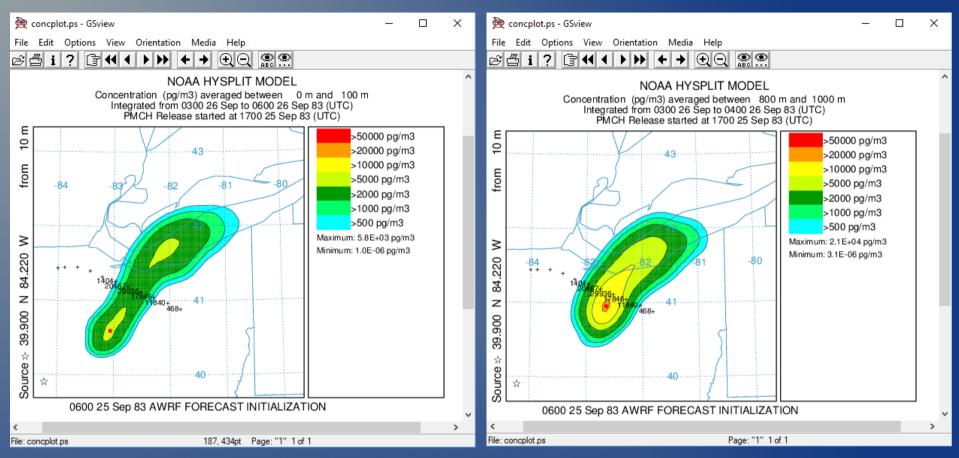
```
captex aircraft level =
                           914 m MSL
year mn dy
            shr
                dur
                        lat
                                lon
                                      pg/m3 plane
1983 09 26 0300 0006 40.86
                             -81.81
                                       468.0
1983 09 26 0300 0006 40.94
                             -82.04 11840.4
                                                 7
1983 09 26 0300 0006 41.02
                             -82.29 17846.4
                                                 7
1983 09 26 0300 0006 41.09
                             -82.52 29936.4
                                                 7
    09 26 0300 0006 41.16
                             -82.75 20467.2
1983 09 26 0300 0006 41.23
                             -82.97
                                     1404.0
    09 26 0300 0006 41.29
                             -83.21
                                         0.0
                             -83.43
                                                 7
1983 09 26 0300 0006 41.37
                                         0.0
                                                 7
                             -83.65
                                         0.0
1983 09 26 0300 0006 41.42
1983 09 26 0300 0006 41.42
                             -83.88
                                         0.0
                                                 7
1983 09 26 0300 0006 41.41
                             -84.00
                                         0.0
```

Configure the HYSPLIT simulation to output air concentrations corresponding with one of the sampling aircraft passes.



9.2 Base Configuration Optimization

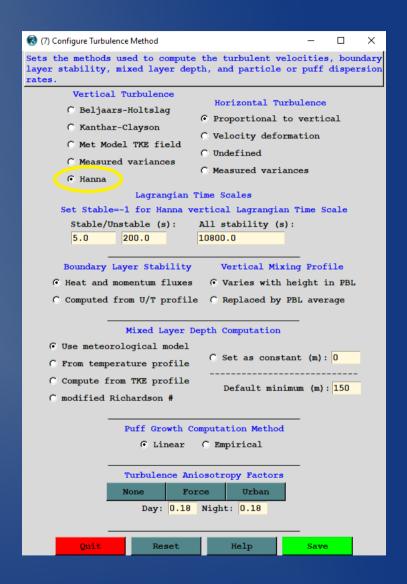
AGL or MSL



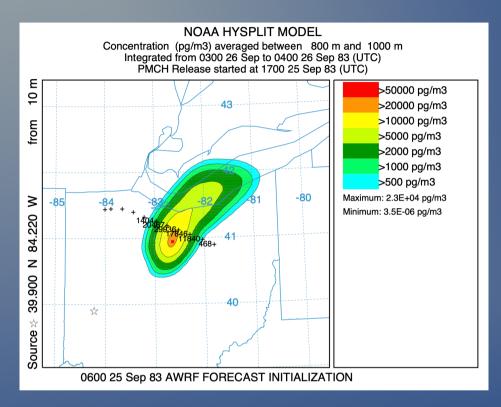
- Finer concentration grid at aircraft sampling level defined in m MSL
- Use horizontal Gaussian particle model for smoother looking results
- Reduced averaging time to more closely match 6 min aircraft collection
- What happens to the tracer release height when units equals MSL?

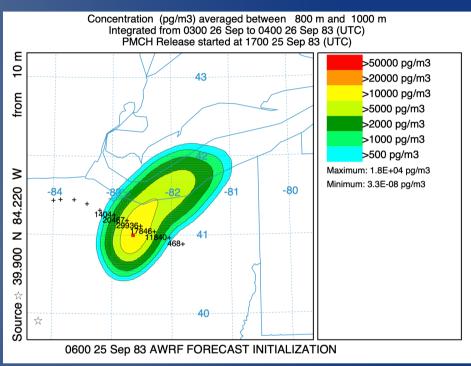
9.3 Turbulence Parameterizations

- Determines how the meteorological data are processed to compute the horizontal and vertical turbulence
- The results shown here provide some rationale for the the default turbulence settings
- Turbulence options are intended to provide some flexibility when using different input meteorological data
- One use shown later is in the development of a physics ensemble
- Most similar, but Hanna variable T_L shows the greatest differences



9.4 Stability Computation Method

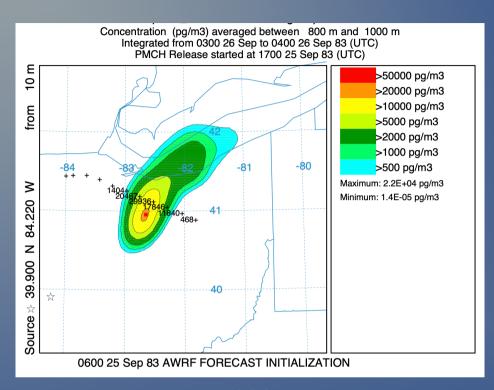


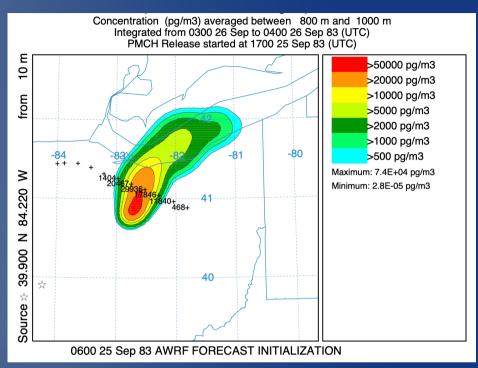


Heat and Momentum Fluxes

Wind and Temperature Profile

9.5 Mixed Layer Depth Calculation





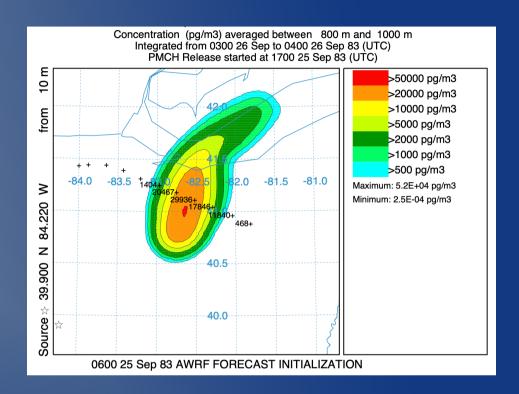
Force to 5000 m

Force to 1250 m

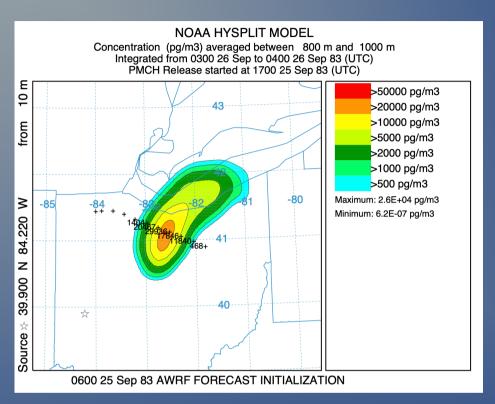
When the PBL is from WRF, T(z), Ri, or fixed at 5000 m, the results are very similar. The air concentration prediction is affected by the mixed layer depth only in situations when the particles interact with this mixing boundary (the forced 1250 m case).

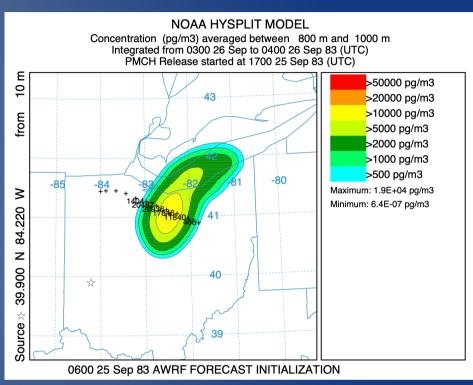
9.6 Turbulent Kinetic Energy

- Defines mixing directly
 - $E = 0.5 (u'^2 + v'^2 + w'^2)$
 - Stability not required
- Need anisotropy factor:
 - $w'^2 / (u'^2 + v'^2)$
 - Default = 0.18
- Why force a value?



9.7 Dispersion Computation Method



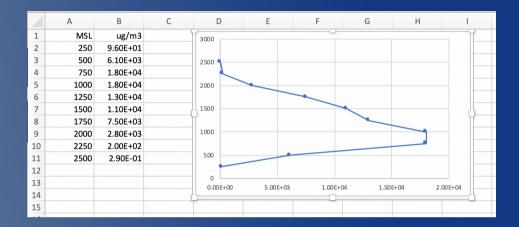


Mass consistent mixing IDSP=2
Best for inverse modeling?

Mass-coupled time averaged winds wvert=.true.

Exercise #9

- Compare first aircraft pass results with second pass
- Determine model concentration profile at location of measured peak

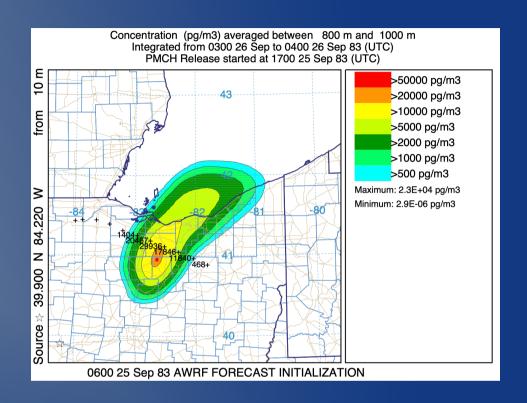


10.1 Display Scripting

```
USAGE: concplot -[options (default)]
  -a[Arcview GIS: 0-none 1-log10 2-value 3-KML 4-partial KML]
 +a[KML altitude mode: (0)-clampedToGround, 1-relativeToGround]
 -A[KML options: 0-none 1-KML with no extra overlays]
 -b[Bottom display level: (0) m]
 -c[Contours: (0)-dyn/exp 1-fix/exp 2-dyn/lin 3-fix/lin 4-set 50-0,interval 10 51-1,interval 10]
 -d[Display: (1)-by level, 2-levels averaged]
 -e[Exposure units flag: (0)-concentrations, 1-exposure, 2-chemical threshold,
                                3-hypothetical volcanic ash, 4-mass loading]
 -f[Frames: (0)-all frames one file, 1-one frame per file]
 -q[Circle overlay: ( )-auto, #circ(4), #circ:dist km]
 -h[Hold map at center lat-lon: (source point), lat:lon]
 -i[Input file name: (cdump)]
 -i[Graphics map background file name: (arlmap) or shapefiles.<(txt)|process suffix>]]
 -k[Kolor: 0-B&W, (1)-Color, 2-No Lines Color, 3-No Lines B&W]
 -1[Label options: ascii code, (73)-open star]
 +l[Use THIS IS A TEST label: (0)-no, 1-ves]
 -L[LatLonLabels: none=0 auto=(1) set=2:value(tenths)]
 -m[Map projection: (0)-Auto 1-Polar 2-Lamb 3-Merc 4-CylEqu]
 +m[Maximum square value: 0=none, (1)=both, 2=value, 3=square]
 -n[Number of time periods: (0)-all, numb, min:max, -incr]
 -o[Output file name: (concplot.ps)]
 -p[Process file name suffix: (ps) or process ID]
 -q[Quick data plot: ( )-none, filename]
 -r[Removal: 0-none, (1)-each time, 2-sum, 3-total]
 -s[Species: 0-sum, (1)-select, #-multiple]
 -t[Top display level: (99999) m]
 -u[Units label for mass: (mass), see "labels.cfg" file]
 -v[Values[:labels:RRRGGGBBB color (optional, but must have 2 colons to specify color without label)
       for <= 25 fixed contours: val1:lab1:RGB1+val2:lab2:RGB2+val3:lab3:RGB3+val4:lab4:RGB4]
 -w[Grid point scan for contour smoothing (0)-none 1,2,3, grid points]
 -x[Concentration multiplier: (1.0)]
 -v[Deposition multiplier:
                               (1.0)
 -z[Zoom factor: 0-least zoom, (50), 100-most zoom]
 -1[Minimum concentration contour value when -c=0 or 1: (0.0)-none, ()-value]
 -2[Minimum deposition contour value when -c=0 or 1: (0.0)-none, ()-value]
 -3[Allow colors to change for dynamic contours (-c=0 or 2): (0)-no, 1-ves]
 -4[Plot below threshold minimum contour for chemical output (-e=2): (0)-no, 1-yes]
 -5[Use -o prefix name for output kml file when -a=3 or 4: (0)-no, 1-yes]
 -8[Create map(s) even if all values zero: (0)-no, 1-ves]
 -9[Force sample start time label to start of release: (0)-no, 1-yes]
```

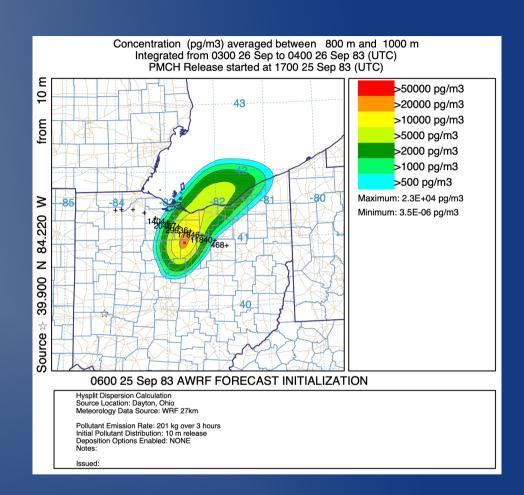
10.2 County Map Boundaries

- Requires: shapefiles.txt
- File name, line spacing, thickness, RGB
- '/Tutorial/maps/roads.shp'0 0.005 0.8 0.7 0.5
- '/Tutorial/maps/county.shp' 0 0.010 0.4 0.6 0.8
- '/Tutorial/maps/states.shp' 0 0.015 0.2 0.2 0.5
- Edit for UNIX: ~/Tutorial/...



10.3 Enhanced Graphic Labels

- Panel label requires:MAPTEXT.CFG
 - Not all lines transferred to the graphic
 - Displayed lines depend upon the graphic type
- Border label: requiresLABELS.CFG



10.4 Creating KML/KMZ for GE

- The display radio-button creates a "KMZ" file which is just a zip file containing the contours in HYSPLIT_ps.kml and various logos and labels
- The HYSPLIT GUI cannot open Google Earth internally as an application
- Go to the \working directory and open the "KMZ" file
- If the "KMZ" file has not been created, the uncompressed "KML" file should still be available for display

10.5 Creating HYSPLIT Shapefiles

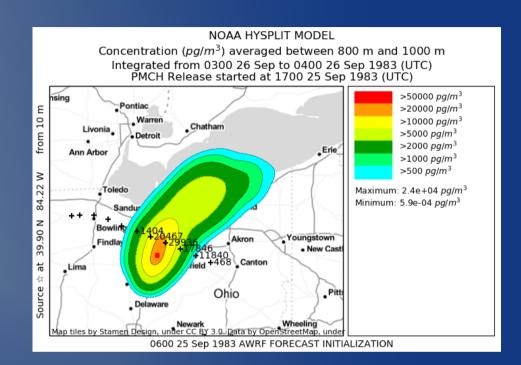
- The plotting program requires an option to create an output file in ESRI generate format (most use either -a or -g)
- GNU utility programs are used to convert the generate format file to a points, line, or polygon shapefile
- Four output files will be created (*.shp, *.shx, *.dbf, *.prj)

10.6 Shapefile Overlays

 Those shapefiles can then be displayed in any HYSPLIT plotting program as an additional map background file (shapefiles.txt)

10.7 Python Display Options

- Need a Python emulator, e.g. Anaconda
- Available for trajplot, concplot, and toaplot – uses the same command line options
- Multiple output formats available: pdf, png, ...
- Simple, city, or terrain map backgrounds



11.1 Linear Mass Conversions

Day/Time	Base	POL1	POL2
25/18-21	48000	39000	8300
25/21-00	36000	24000	12000
26/00-03	18000	9300	8200
26/03-06	6400	2200	4300
26/06-09	9000	2300	6700
26/09-12	6500	1300	5200
26/12-15	2600	380	2200
26/15-18	1600	170	1400

Maximum concentrations for no conversion (base) and 10% per hour from pollutant #1 to pollutant #2

The conversion option is not intended to replace the need for non-linear chemical models, but to provide some guidance as to the potential effect of first-order transformations.

ICHEM=2 automatically sets MAXDIM=2 to put new mass on different particles.

Total mass is the same as the no transformation simulation.

11.2 Dry Deposition of Gases

- $V_d = D_{dry} / C$
- $\beta_{\rm dry} = V_{\rm d} \Delta Z_{\rm sfc}^{-1}$
- D_{total} = m {1-exp[- Δ t (β_{dry} + β_{wet} + $\beta_{...}$)]}
- In the example calculation, $V_d = 0.01 \text{ m/s}$

After 25 h, 14% of the mass is lost to deposition, and the maximum concentration decreased by 20%

11.3 Dry Deposition of Particles

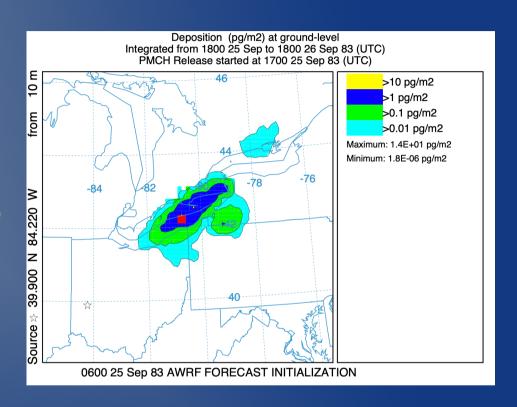
 $Vg = d_p^2 g (\rho_g - \rho) (18 \mu)^{-1}$

Day/Time	Base	Gas	Part	Prob
25/18-21	48000	41000	52000	51000
25/21-00	36000	20000	37000	39000
26/00-03	18000	2900	14000	14000
26/03-06	6400	3600	13000	13000
26/06-09	9000	4100	8500	9200
26/09-12	6500	2100	3200	3600
26/12-15	2600	1600	3200	2700
26/15-18	1600	1300	1900	1800

The removal rate (Vd=Vg) is the same as for a gas, but the particles also gravitationally settle. After 25 h, 30% of the mass is lost to deposition, but the maximum concentration is higher than the no-deposition base simulation.

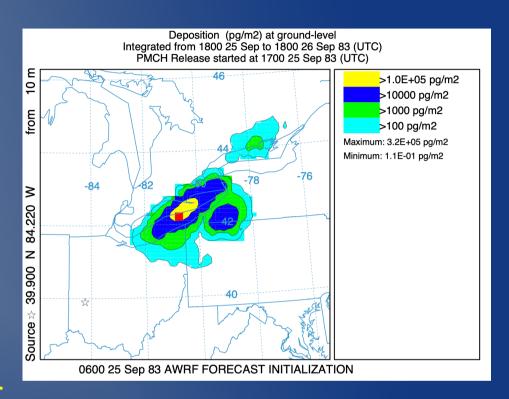
11.4 Wet Deposition for Gases

- V_{gas} = H R T P
- $\beta_{gas} = V_{gas} \Delta Z^{-1}$
- In the example calculation for molecular iodine (H=3.0), only 0.005% of the mass is lost to wet deposition

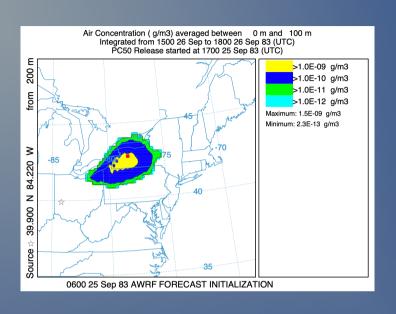


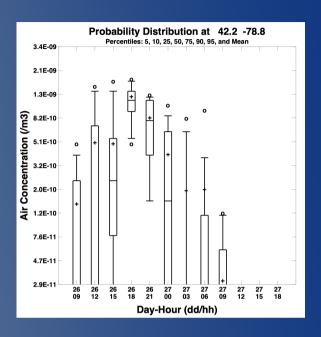
11.5 Wet Deposition for Particles

- $\beta_{\text{wet}} = 8x10^{-5} P^{0.79}$
- The default scavenging coefficient (8x10⁻⁵), applied both below- and within-cloud
- Example mass removed 1 kg
- Deposition 10,000 greater than gaseous wet deposition
- 200 kg evenly deposited over the earth = 400 pg/m²



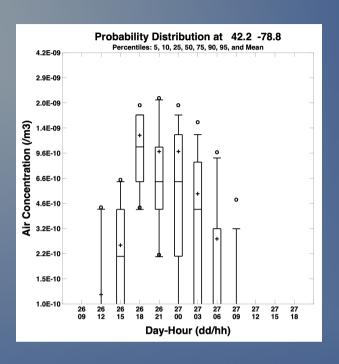
12.1 Meteorological Grid Ensemble

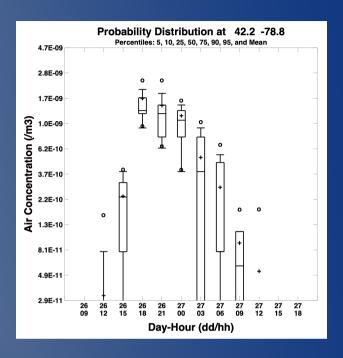




- Shows how results are sensitive to the meteorology data grid
- Similar to the trajectory ensemble, but results are output to 27 concentration files with suffixes 001 through 027
- Post-processing step sorts member results for each grid point and creates probability, mean, and variance output files
- Large range at early and later times due to many members having zero values

12.2 Turbulence and 12.3 Physics Ensembles

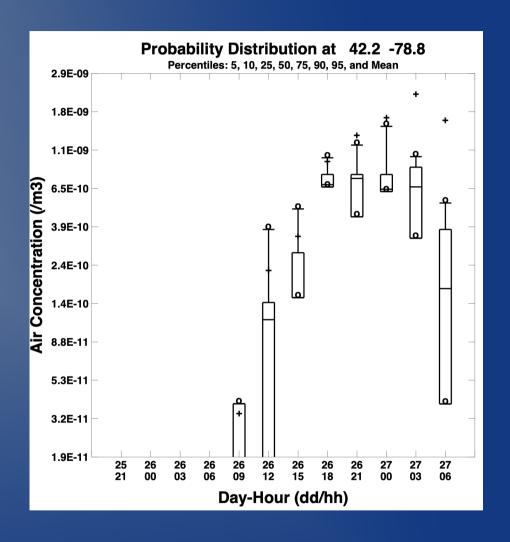




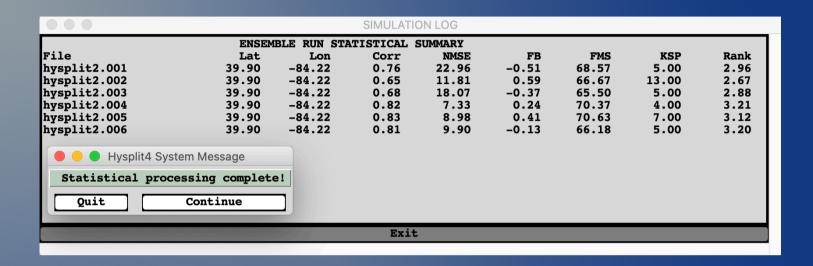
- Turbulence ensemble uses a random seed and reduced particle number (1/27) to estimate uncertainty; alternate approach krand=4
- Physics ensemble reruns the simulation 15 times, each with different turbulence and stability parameterizations
- In both cases, the uncertainty less than grid ensemble

12.4 Multiple Meteorology Ensemble

- Five output files: capex2_{...}
 - 1. wrf27uw.bin
 - 2. era40.bin
 - 3. narr.bin
 - 4. wrf27.bin
 - 5. wrf09.bin
- Results show much tighter distribution than previous ensembles!
- Not sufficiently independent because 3 of 5 members used WRF for the calculation



12.5 Ensemble Verification



- WRF performance better than NARR or ERA
- Ensemble mean (006) similar to the best model (004)
- Suggests care required in selecting ensemble members

12.6 Ensemble Reduction Techniques

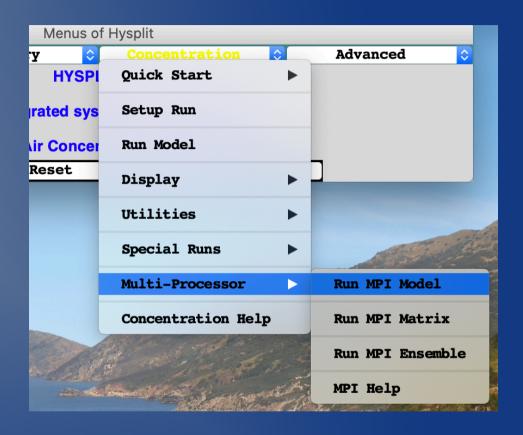
- All member combinations are compared with measurements to find the one with the the minimum RMSE: #2 = (1 + 5)
- Objective is to eliminate members that are not much different from each other, to reduce ensemble mean bias

```
5 files
 Opened
Group #:
 possible combinations:
min. Square Error 1.9677528E+06
group members:
Group #:
 possible combinations:
                                 10
min. Square Error 1.3705874E+06
aroup members:
Group #:
 possible combinations:
                                 10
min. Square Error 1.4504059E+06
aroup members:
Group #:
 possible combinations:
min. Square Error 1.4938470E+06
group members:
Group #:
 possible combinations:
min. Square Error 1.4618720E+06
group members:
```

- In forecast applications: update each analysis cycle with new data and use the best ensemble for the next forecast
- Without data: reduction techniques can also be used to compare members to reduce redundancy

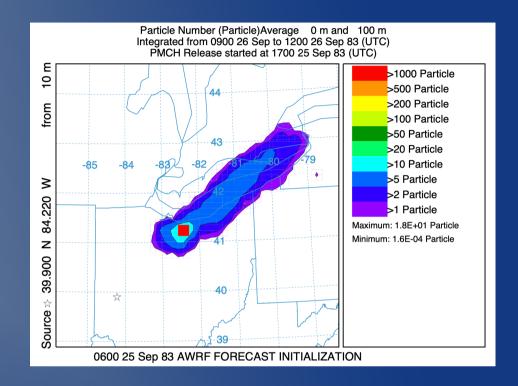
Exercise #12 Problem #3

- OpenMP GEM code only
- MPI Special LINUX compilation (MPICH library)
- Multiple serial executions all systems
- Multiple executions from a single directory



13.1 Counting Particle Trajectories

- Each particle has mass of 1.0
- Particle intersections sum on the concentration grid
- Results are not divided by the grid cell volume
- Output files are manipulated with the concentration utilities



- Results are related to the trajectory frequency plot with residence time on
- However, unlike the mean wind only trajectories, includes stability effects
- Particle count results should be similar to the center-of-mass trajectories

13.2 Emissions from a Known Location

- For CAPTEX: emissions in g/h, measurements in pg/m³
- The measured concentration (M) represents the product of the atmospheric dilution (D) from the source to the receptor and the emission rate (Q):

```
M [g/m^3] = D [h/m^3] Q [g/h]
```

If the emission rate is unknown but the location is known, and the calculation uses a unit emission rate, then the model computes the dilution factor, re-arrange the equation, and adjust for units:

 $Q [g/h] = M [pg/m^3] / (D [hr/m^3] * 1E+12 [pg/g])$

13.3 Backward vs Forward Dispersion

- If multiple receptor stations exist, the "upwind" plumes can be used to triangulate a source region
- The emission can be estimated, if the dispersion from the receptor to source is assumed to be the same as from source to receptor
- There is additional uncertainty in these calculation
- In this example the dispersion rates differ by a factor of 3
- The primary reason is because dispersion is always calculated "forward" regardless of the direction of the advection and turbulence has memory because

$$U'(t+\Delta t) = R(\Delta t) U'(t) + ...$$

13.4 Simulations from Multiple Samplers

- Backward calculations automatically configured in pre-processor step from sampling data file in DATEM format
- In this CAPTEX example, the multiple simulations shown are not ideal for triangulation because of near constant wind direction
- In the "numerator" case the backward calculation emission rate is equal to the measured value giving more weight to the source regions contributing to the highest measurements
- For the inverse case, the calculation emission rate is set to the inverse of the measurement (1/M)
 - From before, M=DQ, the model computes C=DQ
 - If Q is set to 1/M, the the model computes D/M
 - Then the model output is the same as 1/Q
- As the dilution increases (<<D), the emission rate must increase to maintain the same measurement, hence other engineering information can be used to estimated the maximum emission rate possible and hence the contour the limits the emission regions

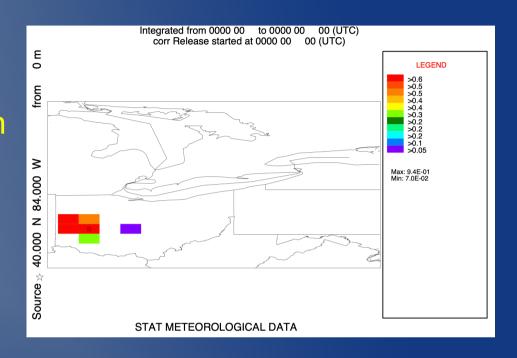
13.5 Source-Receptor Matrix

Г		Α	В	С	D	Е	F	G	
Ш	1		Receptor 1	Receptor 2	Receptor 3		Receptor M		
Ш	2	Source 1 -						Rm from \$1	
Ш	3	Source 2 -						Rm from S2	
Ш	4	Source 3 -						Rm from \$3	
Ш	5							۸.	
н	6	Source N						Air Concentration	
Ш	7		Sn to R1	Sn to R2	Sn to R3				
	8		Source	Sensitivity N	Иaps			Maps	

- Set a switch (ichem=1) so that each source location has its own concentration grid; Multiple sources run simultaneously
- Model output results are treated as a matrix
 - Each row represents a source, a concentration grid cell per column
 - Each column is a grid cell, the row shows the concentration contribution from each source to that location
- Post-processing output options are standard concentration maps for a source or source-location maps for each receptor

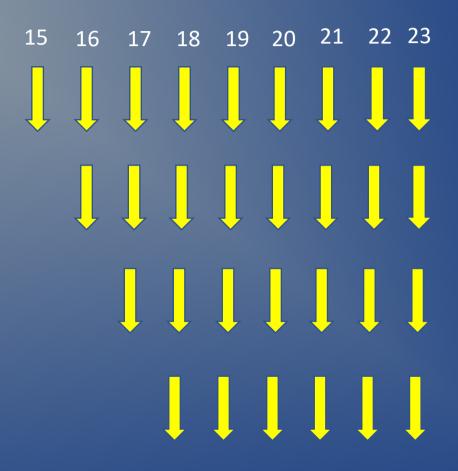
13.6 Source Location Statistics

- Application uses the matrix source results to find which location gives the best fit with the measured data
- Any one of 6 statistical metrics can be chosen to determine the best fit



13.7 Solving the Coefficient Matrix

A Matrix can be defined in space, time, or both



Solving the Coefficient Matrix

\mathbb{Z}	Α	В	С	D	E	F	G	Н	1	J
1	9/25/83 15:00	9/25/83 15:59	9/25/83 17:00	9/25/83 18:00	9/25/83 18:59	9/25/83 20:00	9/25/83 21:00	9/25/83 21:59	9/25/83 23:00	9/26/83 0:02
2	6.32E-02	3.35E-03	0.00E+00	0.00E+00						
3	0.00E+00	6.47E-03	2.16E-03	3.83E-03	9.58E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4	0.00E+00	0.00E+00	1.08E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.86E+02
5	4.46E-02	2.08E-02	8.25E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.56E+03
6	1.06E-01	1.53E-02	2.87E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.12E+01
7	9.58E-04	0.00E+00	1.44E-03	1.34E-02	1.15E-02	6.71E-03	2.88E-03	0.00E+00	0.00E+00	1.36E+03
8	9.57E-04	2.87E-03	2.87E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.57E+03
9	8.32E-02	1.07E-01	3.92E-02	1.05E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.10E+04
10	2.01E-02	7.66E-03	3.83E-03	1.44E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.12E+01
11	1.92E-03	1.01E-02	1.34E-02	1.87E-02	2.01E-02	2.17E-02	9.58E-03	0.00E+00	0.00E+00	6.35E+03
12	0.00E+00	7.66E-03	2.11E-02	2.63E-02	1.10E-02	1.71E-02	0.00E+00	0.00E+00	0.00E+00	7.53E+03
13	2.68E-02	5.31E-02	4.83E-02	3.49E-02	1.63E-02	1.54E-02	5.98E-03	0.00E+00	0.00E+00	2.46E+04
14	0.00E+00	1.44E-03	0.00E+00	0.00E+00	1.92E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.37E+02
15	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.90E-03	5.95E-04	0.00E+00	0.00E+00	1.56E+02
16	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.78E-03	1.20E-03	0.00E+00	0.00E+00	1.87E+02
17	0.00E+00	0.00E+00	2.40E-03	8.62E-03	1.39E-02	2.55E-02	9.58E-03	0.00E+00	0.00E+00	5.13E+03
18	4.78E-04	4.31E-03	5.74E-03	2.54E-02	4.02E-02	5.31E-02	4.19E-02	0.00E+00	0.00E+00	1.20E+04
19	4.78E-04	3.83E-03	9.56E-03	2.06E-02	3.97E-02	2.56E-02	3.17E-02	0.00E+00	0.00E+00	2.18E+04
20	0.00E+00	2.39E-03	0.00E+00	9.57E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.98E+02
21										

Assume that the concentration at receptor R is the linear sum of all the contributing sources S times the dilution factor D between S and R:

$$D_{ij} S_i = R_j$$

$$S_i = (D_{ij})^{-1} R_j$$

- Example shows hourly sources (15-23 UTC)
- Measurements at 19 locations (last column)

Solving the Coefficient Matrix

Actual Data

Actual Data	
Date,	Result,

Date,	Result,
30584.625,	-1.591E+04,
30584.666,	-5.383E+03,
30584.709,	6.828E+05,
30584.750,	-4.226E+05,
30584.791,	5.424E+05,
30584.834,	-1.720E+05,
30584.875,	1.690E+05,
30584.916,	0.000E+00,
30584.959,	0.000E+00,

Hypothetical Data

Date,	Result,
30584.625,	2.576E+02,
30584.666,	-3.618E+03,
30584.709,	7.966E+04,
30584.750,	5.077E+04,
30584.791,	7.393E+04,
30584.834,	4.500E+03,
30584.875,	-4.552E+03,
30584.916,	0.000E+00,
30584.959,	0.000E+00,

- Difficult to obtain solution due to model errors
- If square matrix, can use Excel to solve
- Correct answer should be: 6.7E+04

13.8 Cost Function Minimization

Cost Function Solution

Hypothetical Data

30584.6250	-2.1574E+03	
30584.6660	1.2455E+04	
30584.7090	2.6393E+04	
30584.7500	3.9375E+04	
30584.7910	5.1610E+04	
30584.8340	6.3270E+04	
30584.8750	7.4548E+04	
30584.9160	8.5617E+04	
30584.9590	9.6612E+04	

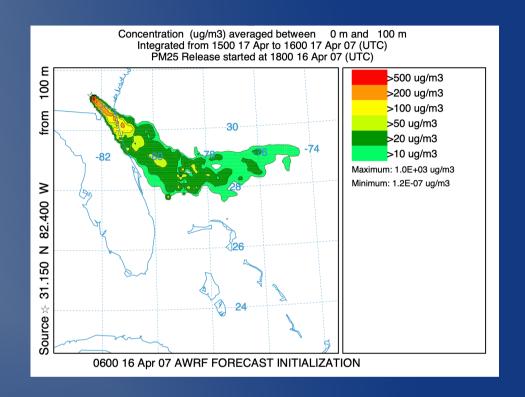
```
Date, Result, 30584.625, 2.576E+02, 30584.666, -3.618E+03, 7.966E+04, 30584.750, 5.077E+04, 30584.791, 7.393E+04, 30584.834, 4.500E+03, 30584.875, -4.552E+03, 30584.916, 0.000E+00, 30584.959, 0.000E+00,
```

- Alternate approach is cost function minimization
- Accounts for model and measurement errors
- The larger the errors, smaller departure from first-guess

$$\mathcal{F} = \frac{1}{2} \sum_{i=1}^{M} \sum_{j=1}^{N} \frac{(q_{ij} - q_{ij}^b)^2}{\sigma_{ij}^2} + \frac{1}{2} \sum_{m=1}^{M} \frac{(a_m^h - a_m^o)^2}{\epsilon_m^2}$$

14.1 Fire Smoke

- Employ USFS tools to determine the emission rate:
 - Blue Sky modeling framework
 - Fire Emission Product Simulator
 - VSMOKE-HYSPLIT interface
- Example uses NOAA's implementation of Blue Sky
- Assumes maximum rate from prescribed burn as the rate from a continuous wildfire



14.2 Dust Storms: Simplified Algorithm

- Vertical dust flux (Q in g) as a fraction of the horizontal transport:
 - Q = $K \rho g^{-1} U_* (U_*^2 U_{**}^2) A$
 - $\mathbf{Q} = 0.01 \mathbf{U}_{\star}^{4} \mathbf{A}$ (simplified)
- Threshold fixed at 28 cm/s
- Over U.S. dust emission
 algorithm needs ½ deg data
- Define 3-point domain
- Run pre-processor step to define desert land-use cells

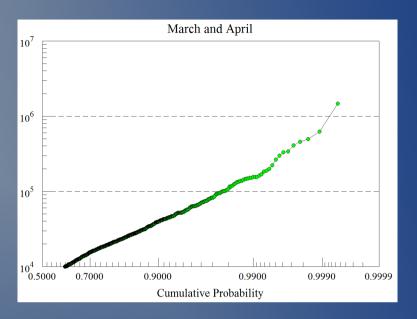
```
CONTROL dust0.txt - Notepad
                                  CONTROL - Notepad
                                  File Edit Format View Help
    Edit Format View Help
                                 10 03 30 00
10 03 30 00
                                   26
                                    40.00
                                            -114.50
                                                               -1.000 0.606F+09
38.00 -115.00
              10.0
                                                       10.
41.00 -110.00
                                            -114.50
                                                       10.
                                                               -1.000 0.606E+09
38.25 -114.75
                                             -114.25
                                                               -1.000 0.606E+09
                                                               -1.000 0.606E+09
                                                               -1.000 0.606E+09
10000.0
                                    38.75
                                            -114.00
                                                       10.
                                                               -1.000 0.606E+09
                                    39.00
                                            -114.00
                                                       10.
                                                               -1.000 0.606E+09
                                    39.25
                                            -114.00
                                                       10.
C:/Tutorial/dust/
                                                               -1.000 0.606E+09
WRF201003.bin
                                    38.50
                                            -113.75
                                                       10.
                                                               -1.000 0.606E+09
                                    38.75
                                            -113.75
                                                               -1.000 0.606E+09
                                                       10.
PM10
                                            -113.75
                                    39.00
                                                       10
                                                               -1.000 0.606E+09
0.0
                                    39.25
                                            -113.75
                                                               -1.000 0.606E+09
30.0
                                            -113.50
                                                               -1.000 0.606E+09
                                            -113.50
00 00 00 00 00
                                                               -1.000 0.606E+09
                                    39.50
                                            -113.50
                                                       10
                                                               -1.000 0.606E+09
0.0 0.0
                                    39.75
                                            -113.50
                                                               -1.000 0.606E+09
                                    40.00
                                            -113.50
0.05 0.05
                                                       10.
                                                               -1.000 0.606E+09
30.0 30.0
                                    40.25
                                            -113.50
                                                               -1.000 0.606E+09
                                    41.00
                                            -113.50
                                                               -1.000 0.606E+09
dust0.bin
                                            -113.25
                                                               -1.000 0.606E+09
                                    39.25
                                            -113.25
                                                               -1.000 0.606E+09
                                                               -1.000 0.606E+09
                                            -113.25
00 00 00 06 00
                                                               -1.000 0.606E+09
                                    40.00
                                            -113.25
                                                       10.
                                                               -1.000 0.606E+09
00 00 00 00 00
00 24 00
                                    40.25
                                            -113.25
                                                       10.
                                                               -1.000 0.606E+09
0.0 0.0
                                    41.00
                                            -113.25
                                                       10.
                                                               -1.000 0.606E+09
                                 30
0.05 0.05
30.0 30.0
                                 10000.0
dust0 byhr.bin
                                 C:\Tutorial\dust\
100
                                 WRF201003.bin
00 00 00 06 00
aa aa aa aa aa
                                 PM10
                                 0.0
00 01 00
0.0 0.0 0.0
                                 00 00 00 00 00
0.0 0.0 0.0 0.0 0.0
```

14.3 Revised Dust Algorithm

- Soil-dust density (K) and emission area (A) are from satellite AOD climatology
 - $Q = K A (U_* U_*^t)$
- Last two columns in CONTROL are U_{*}^t and K A
- Pre-processor not required
- Monthly emission files are provided in the dust directory

```
CONTROL dust2.txt - Notepad
File Edit Format View Help
21
38.50 -114.00 10.0 72.0 0.575E+04
      -113.75 10.0 66.3 0.352E+04
      -113.25 10.0
                    67.4 0.739E+04
      -113.75 10.0
                    74.8 0.166E+05
      -114.00 10.0
                    59.9 0.759F+04
      -113.75 10.0 49.9 0.516E+04
      -113.50 10.0 53.9 0.418E+04
                   76.6 0.535E+04
                    56.7 0.654E+04
39.50 -114.00 10.0
39.50 -113.50 10.0 44.8 0.599E+04
39.50 -113.25 10.0 55.2 0.365E+04
39.50 -113.00 10.0 75.1 0.263F+05
10000.0
C:/Tutorial/dust/
WRF201003.bin
PM10
0.0
30.0
00 00 00 00 00
0.0 0.0
0.05 0.05
30.0 30.0
dust2.bin
```

14.4 Adjusting Emission Factors

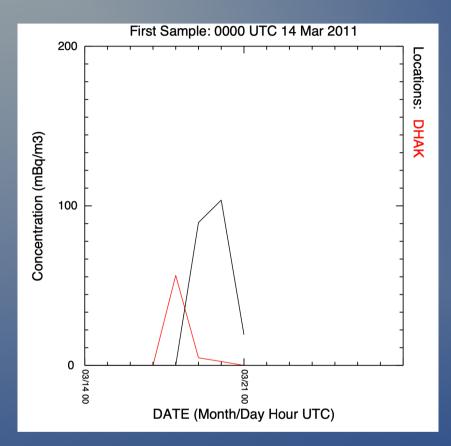


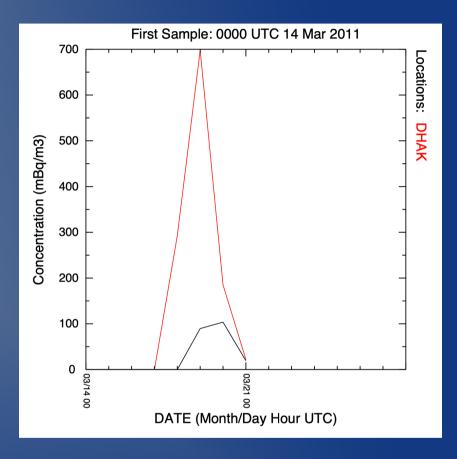
- Dust modeling requires some assimilative techniques
- Emission climatology may not represent current conditions:
 - Recent rain causes crusting and higher thresholds
 - Seasonal rain lack of or excessive vegetation
 - Previous dust storms lack of erodible material
 - Previous flooding events excessive erodible material
- Analyze climatology files to find maximum emission factors
- Adjust threshold velocities as needed to trigger emissions

15.1 Radioactive Decay and Dose

- The mass on a particle is reduced using the time constant approach:
 - $m2 = m1 \exp(-\beta rad \Delta t)$.
- The decay constant is defined by the half-life $(T\frac{1}{2})$:
 - β rad = $\ln 2 / T\frac{1}{2}$
- Doses (either Sv or REM) are computed from published conversion factors, a constant for each radionuclide
 - Airborne: (REM/h) / (Bq/m3).
 - Deposited: (REM/h) / (Bq/m2)
- There are limitations to this simple approach
 - Decay does not start until the particle is emitted
 - For continuous emissions, the rate must be decay corrected
 - Concentration and deposition are decayed during the calculation, but not once written to the output file

15.2 Long-Range I¹³¹ from Fukushima 2.5 deg – 6 h 0.5 deg – 3 h





- Assume that most of the I-131 emissions occurred during the venting and explosion at Unit #2 for 24 h from 1200 UTC on March 14th 2011
- The total I-131 emitted has been reported to be about 150 PBq, which converts to an hourly rate of about 5 PBq

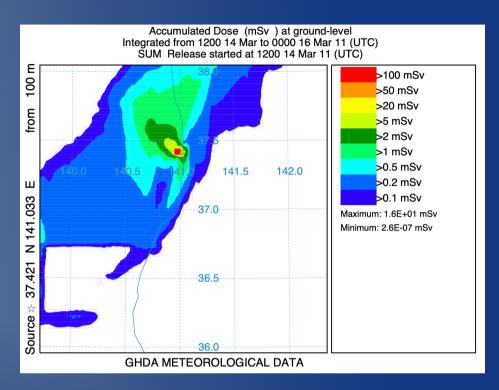
15.3 Dose Calculations from Fukushima

- Configure the model for two surrogate species
 - Non-depositing noble gas (NGAS)
 - Depositing small particle (RNUC)
- Assign both to the same computational particle
- Run the dispersion/deposition for a continuous emission using a unit source and NO decay!
- Concentration, deposition, and radioactive decay are computed in the post-processing step (pgm = con2rem)
 - $C_{j,k,m} = \Sigma [Q_{i,m} D_m TCM_{i,j,k,m}]$
 - And time=i, species=m, decay=D, TCM=dilution, sampler location=k, sampling time=j

Dose Calculations from Fukushima

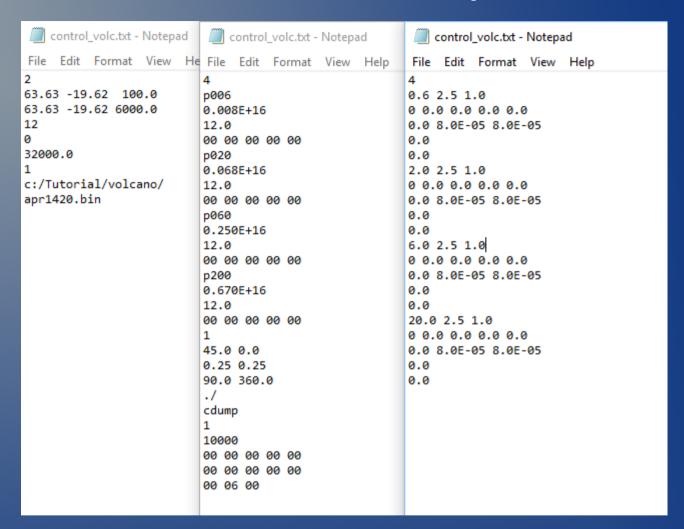
,comp											_
a	ctivity.	txt - Note	pad							_	
File	Edit	Format	View	Help							
Mass	Nucl		T1/2	U235H	U235T	Pu239H	Pu239T	Cloudshine	Groundshine	Inhalati	on
Hr=	0.00)	sec	Bq	Bq	Bq	Bq	rem/h Bq/m3	rem/h Bq/m2	rem/Bq	
95	Nb	3.0200	00E+06	1.62000E+13	1.62000E+13	1.62000E+13	1.62000E+13	1.26000E-08	2.62000E-10	2.38000E	-06
110	Ag	2.1800	0E+07	6.48000E+12	6.48000E+12	6.48000E+12	6.48000E+12	4.57000E-08	9.29000E-10	2.38000E	-06
132	Te	2.8200	0E+05	1.62000E+16	1.62000E+16	1.62000E+16	1.62000E+16	3.36000E-09	7.63000E-11	7.38000E	-07
131	I	6.9465	6E+05	8.10000E+15	8.10000E+15	8.10000E+15	8.10000E+15	6.08400E-09	1.31040E-10	7.38000E	-07
133	I	7.4900	0E+04	8.10000E+15	8.10000E+15	8.10000E+15	8.10000E+15	9.94000E-09	2.22000E-10	7.38000E	-07
133	Xe	4.5299	5E+05	3.66000E+17	3.66000E+17	3.66000E+17	3.66000E+17	5.00400E-10	0.00000E+00	0.00000E	+00
134	Cs	6.5000	0E+07	8.10000E+14	8.10000E+14	8.10000E+14	8.10000E+14	2.54000E-08	5.33000E-10	4.63000E	-07
137	Cs	9.5209	3E+08	8.10000E+14	8.10000E+14	8.10000E+14	8.10000E+14	3.34080E-11	1.07640E-12	4.63000E	-07
140	Ba	1.1016	0E+06	4.05000E+13	4.05000E+13	4.05000E+13	4.05000E+13	2.90520E-09	6.84000E-11	1.03000E	-07
140	La	1.4497	9E+05	4.05000E+13	4.05000E+13	4.05000E+13	4.05000E+13	3.99600E-08	7.77600E-10	1.07000E	-07

- In post processing step each radionuclide in activity file is assigned a surrogate species
- Total air and ground dose computed
 REM (1) or Sieverts (0.01 or 10 mSv)
- Activity file can be modified for each phase of the accident
- No limit to the number of radionuclides assigned
- 3D particle near source results are sensitive to grid size



Note the dependence of deposition to the resolution of the precipitation field

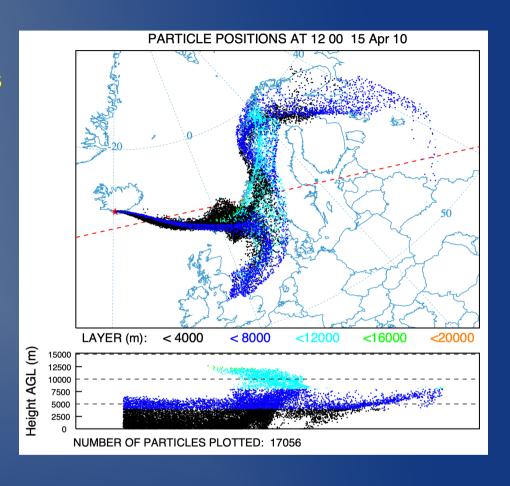
16.1 Volcanic Eruptions



Objective is to create a CONTROL file for a vertical line source with four different particle sizes, each with different emission rates

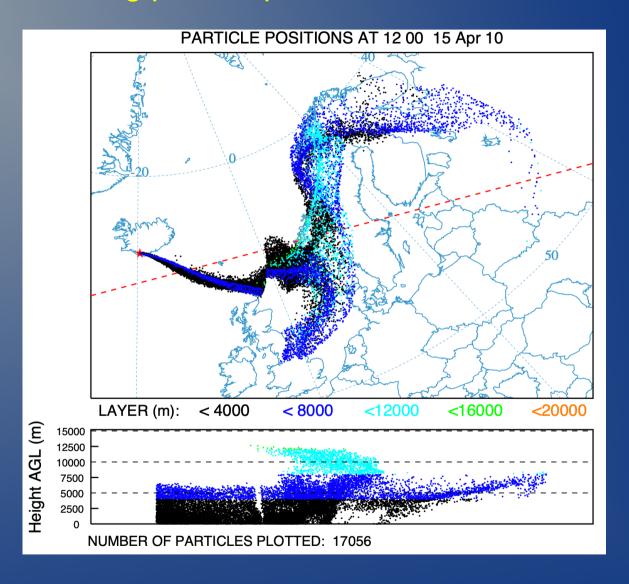
16.2 Restarting the Model from PARDUMP

- Objective is to run two more 12 h simulations with different emissions
- Rename PARDUMP from last simulation to PARINIT
- Reconfigure new emissions to 12 km for the next run
- Restart the model with previous particles emitted to 6 km
- Continue for another 12 h emission cycle but release to only 6 km

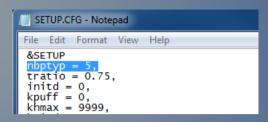


16.3 Assimilation of Satellite Data

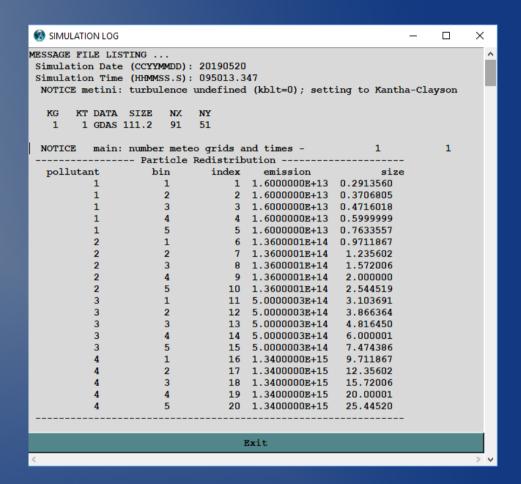
Matching particle positions to observations



16.4 Particle Size Distributions



- Create NBPTYP number of bins for each particle size
- Bin sizes increase by dV/d(log R)
- CONTROL file sizes should be sorted by increasing size



16.5 Creating a complex EMITIMES

```
YYYY MM DD HH
                 DURATION(hhhh) #RECORDS
YYYY MM DD HH MM DURATION(hhmm) LAT LON HGT(m) RATE(/h) AREA(m2) HEAT(w) Emission record description
2010 04 14 00 0012 8
                                                           First emission time group header record
2010 04 14 00 00 1200 63.63 -19.62
                                      100.0 0.01 0.0 0.0
                                                               Emission record height 1, pollutant 1
2010 04 14 00 00 1200 63.63 -19.62 100.0 0.07 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 100.0 0.25 0.0 0.0
                                                               Emission record height 1, pollutant 4
2010 04 14 00 00 1200 63.63 -19.62 100.0 0.67 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.01 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.07 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.25 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.67 0.0 0.0
                                                               Emission record height 2, pollutant 4
```

- Configure three 12 h simulations into one 36 h simulation
- Create EMITIMES file for emissions
- Set emissions to zero in CONTROL

```
LABEL Diameter Percent Release Rate
                     0.008E+16
P006
      0.6µm
              1%
              7%
P020
      2.0µm
                     0.068E+16
      6.0um
              25%
                     0.250E+16
P060
      20.0µm 67%
                     0.670E+16
P200
```

```
EMITIMES - Notepad
File Edit Format View Help
                 DURATION(hhhh) #RECORDS
YYYY MM DD HH
YYYY MM DD HH MM DURATION(hhmm) LAT LON HGT(m) RATE(/h)
2010 04 14 00 0012 8
2010 04 14 00 00 1200 63.63 -19.62 100.0 0.01 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 100.0 0.07 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 100.0 0.25 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 100.0 0.67 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.01 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.07 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.25 0.0 0.0
2010 04 14 00 00 1200 63.63 -19.62 6000.0 0.67 0.0 0.0
2010 04 14 12 3012 8
2010 04 14 12 00 1200 63.63 -19.62 100.0 0.01 0.0 0.0
2010 04 14 12 00 1200 63.63 -19.62 100.0 0.07 0.0 0.0
2010 04 14 12 00 1200 63.63 -19.62 100.0 0.25 0.0 0.0
2010 04 14 12 00 1200 63.63 -19.62 100.0 0.67 0.0 0.0
2010 04 14 12 00 1200 63.63 -19.62 12000.9 0.01 0.0 0.0
2010 04 14 12 00 1200 63.63 -19.62 12000.0 0.07 0.0 0.0
2010 04 14 12 00 1200 63.63 -19.62 12000.0 0.25 0.0 0.0
2010 04 14 12 00 1200 63.63 -19.62 12000.5 0.67 0.0 0.0
2010 04 15 00 0012 8
2010 0 1 15 00 0 1200 63.63 -19.62 100.0 0.01 0.0 0.0
2010 04 15 00 00 1200 63.63 -19.62 100.0 0.07 0.0 0.0
2010 04 15 00 00 1200 63.63 -19.62 100.0 0.25 0.0 0.0
2010 04 15 00 00 1200 63.63 -19.62 100.0 0.67 0.0 0.0
2010 04 15 00 00 1200 63.63 -19.62 6000.0 0.01 0.0 0.0
2010 04 15 00 00 1200 63.63 -19.62 6000.0 0.07 0.0 0.0
2010 04 15 00 00 1200 63.63 -19.62 6000.0 0.25 0.0 0.0
2010 04 15 00 00 1200 63.63 -19.62 6000.0 0.67 0.0 0.0
```

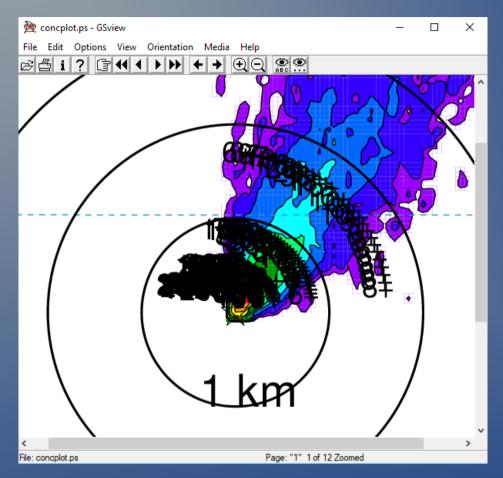
17.1 Dynamic or Lagrangian Sampling

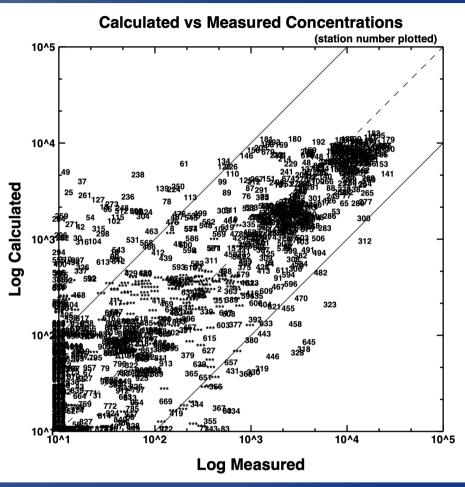
- Rather than a fixed concentration grid, the model can be configured with a sampler that moves through the computational domain
- Dynamic option defines an aircraft which has a prescribed height, direction and speed
- Lagrangian can be considered like a balloon that moves passively with the wind at its prescribed height
- Output is written to a special text file
- No graphics options are available

17.2 Volume or Mass Mixing Ratios

- Default HYSPLIT output in mass/volume units
- Many air pollutant measurements are given in volume mixing ratios (volume pollutant / volume air)
- To convert between units requires the pollutant's molecular weight
- A HYSPLIT shortcut is to divide the output concentration by the air density (ichem=6)
- The resulting output is then mass mixing ratio (mass pollutant / mass air)
- Multiply this result by the ratio of the molecular weight of air (29) to that of the pollutant to get the volume mixing ratio

17.3 Short-Range Dispersion Simulations

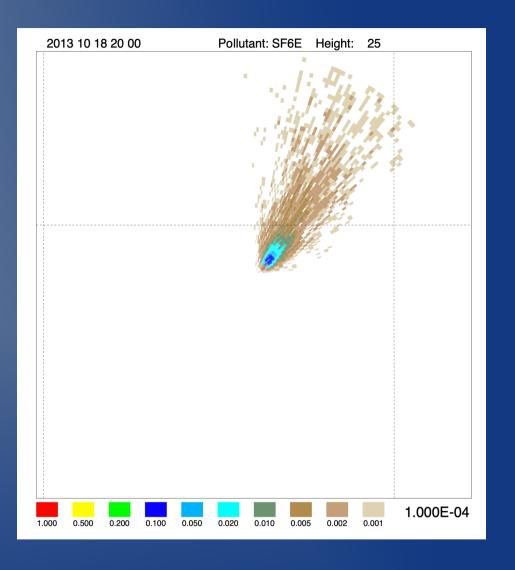




- When a time step of less than 1 min is required, a special code section is invoked to linearly interpolate the particle positions to the concentration grid
- Another option is to use puff rather than particle dispersion to reduce artificial diffusion.

17.4 Polar Coordinate Concentration Grid

- Grid defined in terms of distance and angle from the source
- Requires namelist variable:
 - cpack = 3
- Grid definition becomes:
 - 1.0 0.1 angle & spacing
 - 360.0 5.0 domain & range



17.5 Configuring STILT options in HYSPLIT

$$f(\mathbf{x}_r, t_r | x_i, y_j, t_m) = \frac{m_{\text{air}}}{h\overline{\rho}(x_i, y_j, t_m)} \frac{1}{N_{\text{tot}}} \sum_{p=1}^{N_{\text{tot}}} \Delta t_{p,i,j,k}.$$

Calculates a footprint field [ppm/(micro-mole/m2/s)] to represent the flux, where m is the molar mass of air, ρ is the average density below h, and h is half the mixed layer depth. The summation represents the time that N particles spends in the lower half of the mixed layer.

STILT MODE	ICHEM=8			
Mass consistent dispersion	IDSP=2			
Hanna turbulence equations	KBLT=5			
Modified Richardson number	KMIXD=3			
Variable Lagrangian time scale	VSCALES=-1.0			
Grell convective mixing	CAPEMIN=-2.0			